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Rapid solution of first kind boundary integral equations in $\mathbb{R}^3$*

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Abstract

Weakly singular boundary integral equations (BIEs) of the first kind on polyhedral surfaces Γ in $\mathbb{R}^3$ are discretized by Galerkin BEM on shape-regular, but otherwise unstructured meshes of meshwidth h. Strong ellipticity of the integral operator is shown to give nonsingular stiffness matrices and, for piecewise constant approximations, up to $O(h^3)$ convergence of the farfield. The condition number of the stiffness matrix behaves like $O(h^{-1})$ in the standard basis. An $O(N)$ agglomeration algorithm for the construction of a multilevel wavelet basis on Γ is introduced resulting in a preconditioner which reduces the condition number to $O(|\log h|)$. A class of kernel-independent clustering algorithms (containing the fast multipole method as special case) is introduced for approximate matrix-vector multiplication in $O(N(\log N)^3)$ memory and operations.

Iterative approximate solution of the linear system by CG or GMRES with wavelet preconditioning and clustering-acceleration of matrix-vector multiplication is shown to yield an approximate solution in log-linear complexity which preserves the $O(h^3)$ convergence of the potentials. Numerical experiments are given which confirm the theory.

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1 Introduction

The discretization of integral operators such as

$$(Au)(x) = \int k(x,y)\, u(y)\, d\mu(y) \tag{1.1}$$

by Galerkin-, Collocation or Nyström methods with N degrees of freedom leads to moment matrices $\boldsymbol{A}$ of size $N \times N$ which are fully populated. Therefore, the approximate solution of integral equations

$$Au = f \tag{1.2}$$

becomes prohibitively expensive for large N. The kernel function $k(x,y)$ is often the fundamental solution of an elliptic operator with constant coefficients and hence analytic in $x, y \in \mathbb{R}^d$, $x \neq y$. This fact has been used since the appearance of the Fast Multipole Methods (FMM) by Rokhlin and Greengard ([1], [26] and the references there) in various "fast" algorithms. These algorithms reduce the complexity of the matrix vector multiplication $\underline{x} \longmapsto \boldsymbol{A}\underline{x}$ from N^2 to $O(N(\log N)^a)$ operations for some (small) $a \geq 0$. We mention here only the panel-clustering [14, 15] and wavelet-based methods (see [4, 30] for surveys and [18, 19] for algorithmic aspects of wavelet algorithms). All these algorithms can be viewed as matrix-compression techniques, where the $N \times N$ matrix $\boldsymbol{A}$ is replaced by an approximation $\widetilde{\boldsymbol{A}}$ which is described by $O(N(\log N)^b)$ essential parameters. In the context of (1.2), this replacement generates a consistency error in the approximate solution of (1.2) and therefore must be controlled in terms of the discretization error. Such error analysis has been given for clustering in [15] and for wavelets in [6, 24, 30] and the references there. Fast matrix vector multiplication is ideally suited for iterative solution of linear equation systems by eg. GMRES or CG. For integral equations (1.2) with operators A of the second kind, the condition number of the moment matrix is often bounded independently of N. The error in GMRES or CG iteration ℓ therefore decreases geometrically like q^ℓ with $q < 1$ independent of N and the number ℓ of iterations needed to match the discretization error of $O(N^{-\lambda})$, $\lambda > 0$, behaves like $\ell \gtrsim O(\log N)$, since then $q^\ell < N^{-\lambda}$. With work of $O(N(\log N)^a)$ per iteration, an overall algorithm of log-linear complexity results.

For first kind equations (1.2), the situation is less favorable. Here, the condition of $\boldsymbol{A}$ behaves often like $O(N^{-\mu})$ for some $\mu > 0$ and hence $q \sim 1 - O(N^{-\mu})$, therefore the number ℓ of iterations increases algebraically in N, spoiling log-linear complexity. Consequently, some form of preconditioning is required. Wavelets allow naturally for preconditioning in $H^{\frac{1}{2}}(\Gamma)$, $H^{-\frac{1}{2}}(\Gamma)$ on polyhedral surfaces $\Gamma \subset \mathbb{R}^3$. However, in order to achieve bounded condition numbers for $\boldsymbol{A}$, rather sophisticated constructions of wavelets had to be performed (see [5]), which assure $H^{\pm\frac{1}{2}}(\Gamma)$ norm stability as well as sufficient vanishing moments for matrix-compression. Here, we propose a different approach. We consider Galerkin BEM for weakly singular single layer potential and the simplest, piecewise constant shape functions. It was shown by Oswald in [21] how to obtain in this case a preconditioner in $H^{-\frac{1}{2}}(\Gamma)$ which reduces the condition number of $\boldsymbol{A}$ to $O(\log N)$. While not uniformly bounded, this suffices to reduce the iteration count of iterative solvers to a polylogarithmic function of N. The preconditioner is based on Haar-Wavelets which lack vanishing moments for optimal matrix compression [30]. We therefore

propose to use multipole type methods for this purpose, resulting in algorithms of log-linear complexity for weakly singular integral equations.

Multiple acceleration has at first sight 2 disadvantages as compared to wavelet-based compression. First, classical fast multipole is fairly kernel specific in that particular farfield expansions of kernels $k(x,y)$ of interest have to be derived, whereas wavelet compressions work on large classes of kernels without any explicit analytic kernel information. We overcome this by proposing a new multipole scheme based on kernel interpolation. Second, the Haar-Wavelet preconditioner from [21] assumes a sequence of dyadically refined, nested triangulations on Γ. In practice, however, Γ is often complicated and dyadic refinement is impossible. We generalize [21] by generating wavelet bases on unstructured meshes by recursive agglomeration, as described in [29]. We show that preconditioning based on this agglomeration wavelet basis is effective and yields a log-linear solution algorithm for weakly singular BIEs on unstructured, shape-regular meshes on polyhedra in $\mathbb{R}^3$.

The outline of the paper is as follows: in Chapter 2, we review the Galerkin BEM, Chapter 3 presents a general framework for clustering and estimates the impact of the error introduced by the cluster approximation of the farfield upon the accuracy of the Galerkin solution. Section 4 addresses the agglomeration preconditioner and proves log-linear complexity of the overall algorithm, while Section 5 shows numerical results which confirm the estimates.

2 Model Problem

2.1 Preliminaries

Let $\Omega \subset \mathbb{R}^3$ be a bounded, open polyhedral domain with Lipschitz boundary $\Gamma = \partial\Omega$ which we assume to be a connected union of plane, triangular faces π_j^0, $j = 1, \ldots, N_0$ constituting the mesh $\mathcal{M}^0$ on Γ.

The space $L^2(\Gamma)$ is the space of all functions $u : \Gamma \to \mathbb{C}$ which are square integrable with respect to the surface measure ds. It is a Hilbert space with innerproduct

$$\langle u, v\rangle_0 = \int\limits_{x\in\Gamma} \int\limits_{y\in\Gamma} u(x)\overline{v(y)}\, ds_y\, ds_x \tag{2.1}$$

and norm $\|u\|_{0,\Gamma}^2 = \langle u, u\rangle$. By ∇_Γ, we denote the surface gradient. Then

$$H^1(\Gamma) = \{u \in L^2(\Gamma) : \nabla_\Gamma u \in L^2(\Gamma)^2\} \tag{2.2}$$

is a subspace of $L^2(\Gamma)$. It is a Hilbert space with innerproduct given by

$$\langle u, v\rangle_1 := \langle u, v\rangle_0 + \langle \nabla_\Gamma u, \nabla_\Gamma v\rangle_0 \tag{2.3}$$

and norm given by $\|u\|_{1,\Gamma}^2 = \langle u, u\rangle_1$. By $|u|_{1,\Gamma}$ we mean the seminorm

$$|u|_{1,\Gamma} = \left(\langle \nabla_\Gamma u, \nabla_\Gamma u\rangle_0\right)^{\frac{1}{2}}. \tag{2.4}$$

For $0 < s < 1$, we define $H^s(\Gamma)$ by interpolation: $H^s(\Gamma) = (L^2(\Gamma), H^1(\Gamma))_{s,2}$. It is a Hilbert-space with norm $\|u\|_{s,\Gamma}$ given by

$$\|u\|_{s,\Gamma}^2 = \|u\|_{0,\Gamma}^2 + |u|_{s,\Gamma}^2\,, \quad |u|_{s,\Gamma}^2 = \int\limits_{x\in\Gamma}\int\limits_{y\in\Gamma} \frac{|u(x)-u(y)|^2}{|x-y|^{2+2s}}\, ds_y\, ds_x\,. \tag{2.5}$$

For $-1 \le s < 0$, we define $H^s(\Gamma)$ by duality:

$$H^s(\Gamma) = H^{-s}(\Gamma)^* \tag{2.6}$$

and equip it with norm

$$\|u\|_{s,\Gamma} = \sup_{\varphi\in H^{-s}(\Gamma)} \frac{|\langle\varphi, u\rangle|}{\|\varphi\|_{-s,\Gamma}} \tag{2.7}$$

where $\langle\varphi, u\rangle : H^{-s}(\Gamma)\times H^s(\Gamma) \to \mathbb{C}$ denotes the duality pairing obtained by identifying $L^2(\Gamma)^* = L^2(\Gamma)$ and extending $\langle\cdot,\cdot\rangle_{0,\Gamma}$ to $H^{-s}(\Gamma)\times H^s(\Gamma)$. By γ_0 we denote the trace operator: $\gamma_0 U := U|_\Gamma$ for $U \in C^0(\overline{\Omega})$. It extends to a continuous operator $\gamma_0 : H^{s+\frac{1}{2}}(\Omega) \to H^s(\Gamma)$ for $0 < s < 1$.

2.2 Boundary Integral Equation

In $\Omega^c = \mathbb{R}^3\backslash\overline{\Omega}$, we consider the exterior Dirichlet problem

$$\begin{aligned} P(\partial_x)\, U &= 0 \quad \text{in} \quad \Omega^c\,, \\ \gamma_0\, U &= f \quad \text{on} \quad \Gamma\,, \\ &+ \text{radiation conditions as } |x| \to \infty\,. \end{aligned} \tag{2.8}$$

Here $P(\partial_x)$ is a second order elliptic differential operator in divergence form with constant coefficients, and $f \in H^{\frac{1}{2}}(\Gamma)$ is prescribed boundary data. We denote by $e(z)$ the fundamental solution of $P(\partial_x)$, i.e. $P(\partial_x)\, e(x-y) = \delta(x-y)$. Then the single layer potential Ansatz

$$U(x) = \int\limits_{y\in\Gamma} e(x-y)\,\sigma(y)\, ds_y, \quad x \in \Omega^c \tag{2.9}$$

with unknown density $\sigma \in H^{-\frac{1}{2}}(\Gamma)$ in (2.8) leads to the boundary integral equation

$$V\sigma = f \tag{2.10}$$

where V denotes the weakly singular single layer operator

$$(V\sigma)(x) = \int\limits_{y\in\Gamma} k(x,y)\,\sigma(y)\, ds_y\,, \quad x \in \Gamma\,,$$

with kernel $k(x,y) = e(x-y)$. The Galerkin BEM is based on the variational formulation of (2.10):

$$\sigma \in H^{-\frac{1}{2}}(\Gamma):\ a(\sigma,\sigma^t) = \langle f, \sigma^t\rangle \quad \forall \sigma^t \in H^{-\frac{1}{2}}(\Gamma)\,, \tag{2.11}$$

where the bilinear form $a(\cdot,\cdot)$, given by

$$a(\sigma,\sigma^t) := \langle \sigma^t, V\sigma\rangle = \int\limits_{x\in\Gamma}\int\limits_{y\in\Gamma} k(x,y)\,\sigma(y)\,\overline{\sigma^t(x)}\,ds_y\,ds_x\,,$$

is continuous:

$$\forall \sigma,\sigma^t \in H^{-\frac{1}{2}}(\Gamma):\ |a(\sigma,\sigma^t)| \le \|a\|\,\|\sigma\|_{-\frac{1}{2},\Gamma}\,\|\sigma^t\|_{-\frac{1}{2},\Gamma}$$

and coercive: there is $\gamma > 0$ and a compact form $c(\cdot,\cdot):\ H^{-\frac{1}{2}}(\Gamma)\times H^{-\frac{1}{2}}(\Gamma)\to\mathbb{C}$ such that

$$\forall \sigma \in H^{-\frac{1}{2}}(\Gamma)\ \ Re\, a(\sigma,\sigma) \ge \gamma \|\sigma\|^2_{H^{-\frac{1}{2}}(\Gamma)} - c(\sigma,\sigma)\,. \tag{2.12}$$

We assume in addition that V is injective, i.e. that there are no resonances:

$$\forall \sigma^t : a(\sigma,\sigma^t) = 0 \Longrightarrow \sigma = 0\,. \tag{2.13}$$

Then the problem (2.11) has for every $f \in H^{-\frac{1}{2}}(\Gamma)$, a unique solution and there is $s^*(\Gamma) > 0$ such that

$$\|\sigma\|_{H^{-\frac{1}{2}+s}(\Gamma)} \le C\,\|f\|_{H^{\frac{1}{2}+s}(\Gamma)} \ \text{ for } \ 0 \le s < s^*(\Gamma)\,. \tag{2.14}$$

Example 2.1.

$$\begin{aligned} P(\partial_x)U &= -\Delta U - k^2 U = 0 \quad \text{in} \quad \Omega^c\,,\\ \gamma_0 U &= f \qquad\qquad\qquad\ \ \text{on} \quad \Gamma\,,\\ \frac{\partial U}{\partial r} - ik\,U &= o\Big(\frac{1}{|x|}\Big) \qquad \text{for} \quad |x|\to\infty\,. \end{aligned}$$

Here the fundamental solution is $e(z) = \exp(ik|z|)/(4\pi|z|)$ and (2.12) holds.

2.3 Galerkin Boundary Element Method

From the partition $\mathcal{M}^0$ of Γ a sequence $\{\mathcal{M}^\ell\}_{\ell=0}^\infty$ of meshes is obtained by subdividing recursively each panel $\pi_j^\ell \in \mathcal{M}^\ell$ into 4 congruent subtriangles. Clearly, then

$$h_\ell := \max\{\operatorname{diam}\pi_j^\ell :\ \pi_j^\ell \in \mathcal{M}^\ell\} = 2^{-\ell} h_0\,.$$

With the sequence $\{\mathcal{M}^\ell\}_{\ell=0}^\infty$ of meshes, we associate the spaces of piecewise constant functions

$$V^\ell := \{u \in L^2(\Gamma) :\ u|_{\pi_j^\ell} = \text{const. for } \pi_j^\ell \in \mathcal{M}^\ell\},\ \ \ell = 0,1,2,\ldots\,. \tag{2.15}$$

The Galerkin BEM for (2.11) on V^L for some $L \ge 0$ is:

$$\sigma^L \in V^L :\ a(\sigma^L,\sigma^t) = \langle f,\sigma^t\rangle \quad \forall \sigma^t \in V^L\,. \tag{2.16}$$

For a panel $\pi_j^\ell \in \mathcal{M}^\ell$, denote by $\varphi_j^\ell = |\pi_j^\ell|^{-\frac{1}{2}}\,\chi_{\pi_j^\ell}$ its indicator function. Then $V^\ell = \operatorname{span}\{\varphi_j^\ell\}_{j=1}^{N_\ell}$, $\sigma^L = \sum_{j=1}^{N_L}\sigma_j^L\,\varphi_j^L$ and (2.16) is a linear system for the unknown coefficient vector $\underline{\sigma}^L = \{\sigma_j^L\}_{j=1}^{N_L}$:

$$\boldsymbol{A}^L \underline{\sigma}^L = \underline{f}^L\,, \tag{2.17}$$

with

$$A^L_{ij} = a(\varphi^L_j, \varphi^L_i) = \langle \varphi^L_i, V\varphi^L_j\rangle = |\pi^L_i|^{-\frac{1}{2}}\,|\pi^L_j|^{-\frac{1}{2}} \int\limits_{\pi^L_j}\int\limits_{\pi^L_i} k(x,y)\,ds_y\,ds_x\,,\quad f^L_i = \langle f, \varphi^L_i\rangle\,. \tag{2.18}$$

The subspace sequence $\{V^\ell\}_{\ell=0}^\infty$ is dense in $H^{-\frac{1}{2}}(\Gamma)$. Hence the coercivity (2.12) and the uniqueness (2.13) imply **stability:** there is $\gamma > 0$ and L_0 sufficiently large such that the discrete inf-sup conditions hold:

$$\begin{aligned}
&\forall u^L \in V^L: \quad \sup_{v^L\in V^L} \frac{|a(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \geq \gamma\,\|u^L\|_{-\frac{1}{2},\Gamma}\,,\quad L \geq L_0\,,\\
&\forall v^L \in V^L: \quad \sup_{u^L\in V^L} \frac{|a(u^L, v^L)|}{\|u^L\|_{-\frac{1}{2},\Gamma}} \geq \gamma\,\|v^L\|_{-\frac{1}{2},\Gamma}\,,\quad L \geq L_0\,,
\end{aligned} \tag{2.19}$$

and hence for $L \geq L_0$, the Galerkin solutions σ^L exist, $\boldsymbol{A}^L$ is nonsingular and there is $C > 0$ such that

$$\|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} \leq C \min_{\varphi\in V^L} \|\sigma - \varphi\|_{-\frac{1}{2},\Gamma}\,. \tag{2.20}$$

In particular, we also have stability of the Galerkin solutions

$$\|\sigma^L\|_{-\frac{1}{2},\Gamma} \leq C\,\|f\|_{\frac{1}{2},\Gamma},\quad L \geq L_0\,, \tag{2.21}$$

with C independent of L.

2.4 Convergence Rates

Assuming exact quadrature in (2.18) and exact solution of (2.17), the convergence rate of σ^L as L increases is determined by the regularity (2.14) of σ and the approximation properties of the subspaces V^ℓ. There holds

Proposition 2.2. *For $\ell \geq 0$, let $P_\ell : L^2(\Gamma) \to V^\ell$ denote the $L^2(\Gamma)$-projection, i.e. $\langle u - P_\ell u, \varphi\rangle_0 = 0$ for all $\varphi \in V^\ell$. Then*

$$\|u - P_\ell u\|_{L^2(\Gamma)} \leq C\,h_\ell\,\|\nabla_\Gamma u\|_{L^2(\Gamma)} \tag{2.22}$$

where $C > 0$ depends only on the shape of the $\pi^0_j \in \mathcal{M}^0$.

Proof. We have $\|u - P_\ell u\|^2_{L^2(\Gamma)} = \sum_j \|u - P_\ell u\|^2_{L^2(\pi^\ell_j)}$. On element π^ℓ_j, $P_\ell u = \langle u, \varphi^\ell_j\rangle = \frac{1}{|\pi^\ell_j|}\int_{\pi^\ell_j} u\,ds$, hence Poincaré's inequality on $\pi^0_j \supset \pi^\ell_j$ and a scaling argument give

$$\|u - P_\ell u\|_{L^2(\pi^\ell_j)} \leq C h_\ell\,\|\nabla_\Gamma u\|_{L^2(\pi^\ell_j)}\,.$$

Squaring and summing over all $\pi^\ell_j \in \mathcal{M}^\ell$ gives (2.22). ∎

From (2.22), we get the approximation property of V^ℓ.

Proposition 2.3. *For every $s > 0$, there is $C > 0$ independent of ℓ, such that as $\ell \to \infty$*

$$\min_{\varphi \in V^\ell} \|\sigma - \varphi\|_{H^{-\frac{1}{2}}(\Gamma)} \leq C h_\ell^{\min(s,\frac{3}{2})} \|\sigma\|_{H^{-\frac{1}{2}+s}(\Gamma)} . \tag{2.23}$$

Proof. Let $\sigma \in H^1(\Gamma)$ and $\varphi = P_\ell \sigma \in V^\ell$. Then

$$\begin{aligned} \|\sigma - \varphi\|_{H^{-\frac{1}{2}}(\Gamma)} &= \sup_{\psi \in H^{\frac{1}{2}}(\Gamma)} \frac{\langle \sigma - \varphi, \psi \rangle}{\|\psi\|_{H^{\frac{1}{2}}(\Gamma)}} = \sup_{\psi \in H^{\frac{1}{2}}(\Gamma)} \frac{\langle \sigma - \varphi, \psi - P_\ell \psi \rangle}{\|\psi\|_{H^{\frac{1}{2}}(\Gamma)}} \\ &\leq \|\sigma - \varphi\|_{L^2(\Gamma)} \sup_{\varphi \in H^{\frac{1}{2}}(\Gamma)} \frac{\|\psi - P_\ell \psi\|_{L^2(\Gamma)}}{\|\psi\|_{H^{\frac{1}{2}}(\Gamma)}} . \end{aligned}$$

Now $\|\psi - P_\ell \psi\|_{L^2(\Gamma)} \leq C \|\psi\|_{L^2(\Gamma)}$ and (2.22) give with interpolation

$$\|\psi - P_\ell \psi\|_{L^2(\Gamma)} \leq C h_\ell^{\frac{1}{2}} \|\psi\|_{H^{\frac{1}{2}}(\Gamma)}$$

whence we get, using again (2.22),

$$\|\sigma - P_\ell \sigma\|_{H^{-\frac{1}{2}}(\Gamma)} \leq C h_\ell^{\frac{3}{2}} \|\nabla_\Gamma \sigma\|_{L^2(\Gamma)} .$$

(2.23) now follows by interpolation with (2.21). □

The convergence rate of the Galerkin BEM (2.16) follows from (2.20), (2.23):

Proposition 2.4. *Assume* (2.14). *Then the boundary element solution σ^L in* (2.16) *satisfies for $0 \leq s < s^*(\Gamma)$ the error estimate*

$$\|\sigma - \sigma^L\|_{H^{-\frac{1}{2}}(\Gamma)} \leq C h_L^{\min(s,\frac{3}{2})} \|f\|_{H^{\frac{1}{2}+s}(\Gamma)} . \tag{2.24}$$

Often, the solution σ^L is not of main interest, but rather the farfield $U(x)$ for $x \in \Omega^c$. Given σ^L, we approximate $U(x)$ by

$$U^L(x) := \int_{y \in \Gamma} e(x - y)\, \sigma^L(y)\, ds_y, \quad x \in \Omega^c . \tag{2.25}$$

This approximation converges faster than (2.24) as follows from the following Nitsche duality argument [16]: let $x \in \Omega^c$ and ψ_x solve the adjoint problem

$$\psi_x \in H^{-\frac{1}{2}}(\Gamma) : \ \langle V^* \psi_x, \psi^t \rangle = \langle e(x, \cdot), \psi^t \rangle \quad \forall \psi^t \in H^{-\frac{1}{2}}(\Gamma) . \tag{2.26}$$

Then by (2.25), we have for any $\psi^L \in V^L$

$$\begin{aligned} |U(x) - U^L(x)| &= |\langle e(x, \cdot), \sigma - \sigma^L \rangle| = |\langle V^* \psi_x, \sigma - \sigma^L \rangle| \\ &= |\langle \psi_x, V(\sigma - \sigma^L) \rangle| = |\langle \psi_x - \psi^L, V(\sigma - \sigma^L)| \\ &\leq \|a\| \, \|\psi_x - \psi^L\|_{H^{-\frac{1}{2}}(\Gamma)} \, \|\sigma - \sigma^L\|_{H^{-\frac{1}{2}}(\Gamma)} . \end{aligned}$$

Since $e(x,\cdot)$ is smooth on Γ, $\psi_x \in H^{-\frac{1}{2}+s}(\Gamma)$ for $0 < s \leq s'(\Gamma)$, where $s'(\Gamma)$ is the regularity index for V^*. It follows that as $L \to \infty$

$$|U(x) - U^L(x)| \leq C\, h_L^s,\ 0 \leq s < \min\left\{s^*(\Gamma), \frac{3}{2}\right\} + \min\left\{s'(\Gamma), \frac{3}{2}\right\}. \tag{2.27}$$

Analogously, the well-posedness and the convergence rates of the Galerkin-BEM for $Au = Bf$ resulting e.g. from the direct boundary reduction of elliptic boundary value problems:

$$\sigma^L \in V^L : a(\sigma^L, \sigma^t) = b(f, \sigma^t) \quad \forall \sigma^t \in V^L, \tag{2.28}$$

with $b(f, \sigma^t) = \langle \sigma^t, Bf \rangle$ can be proved.

3 Cluster Methods

The matrix of the linear system (2.17) is ill-conditioned and fully populated. Thus, (2.17) is for large N_L expensive to solve. To reduce the complexity of the equation solution, multipole-type expansions in conjunction with iterative solvers like GMRES or CG are often used. We present here a class of multipole methods which require only the kernel function $k(x,y)$, but not the expansion coefficients and which have similar properties like the fast multipole method. Using this cluster approximation of the far field yields a perturbed matrix $\widetilde{\boldsymbol{A}}^L$ and, consequently, a perturbed boundary element solution $\widetilde{\sigma}^L$ in place of σ^L. We estimate the error $\sigma^L - \widetilde{\sigma}^L$ due to clustering the far field and show that an expansion order $m = O(|\log h_L|)$ is sufficient to preserve the consistency (2.24). We also give a general algorithmic framework which accommodates various multipole-type discretizations. Since the concepts are not restricted to weakly singular operators, we assume a singularity of order $\widehat{s}$. We also present the cluster-algorithms in a more general setting which covers in particular also multipole evaluations of the representation formula or Nyström and collocation discretizations of the operator A.

3.1 Kernel Expansions

Assumption 3.1. *Let $0 \leq \eta < 1$, $k : D \times D \to \mathbb{C}$ a kernel function and $\mathcal{I}$ an index set. Then for all $x_0, y_0 \in D$, $x_0 \neq y_0$, and expansion orders $m \in \mathbb{N}_0$ there exists an approximation k_m of the form*

$$k(x,y) \approx k_m(x,y;x_0,y_0) := \sum_{(\mu,\nu)\in\mathcal{I}_m} \kappa_{(\mu,\nu)}(x_0,y_0) X_\mu(x;x_0) Y_\nu(y;y_0) \tag{3.1}$$

for $\mathcal{I}_m \subset \mathcal{I} \times \mathcal{I}$ such that for all $x, y \in D$ satisfying

$$|y - y_0| + |x - x_0| \quad \leq \quad \eta |y_0 - x_0| \tag{3.2}$$

the error is bounded by

$$|k(x,y) - k_m(x,y;x_0,y_0)| \quad \leq \quad C e^{-C(\eta)m} |y - x|^{-\widehat{s}} \tag{3.3}$$

with $C(\eta) > 0$ a decreasing function and C a constant both independent of m. $\widehat{s}$ denotes the singularity order of the kernel for $x = y$.

The goal of the expansion (3.1) is to decouple the source points y from the field points x. The simplest example of such a decoupling is Taylor expansion.

3.1.1 Taylor Expansion [15]

Let the kernel function k only depend on the difference of its arguments:

$$k(x,y) \;=\; k(y-x). \tag{3.4}$$

We expand $k(y-x)$ formally into a Taylor series centered at $y_0 - x_0$ with $x_0, y_0 \in \mathbb{R}^d$:

$$k(y-x) \;=\; \sum_{(\nu,\mu)\in\mathbb{N}_0^d\times\mathbb{N}_0^d} (D^{\mu+\nu}k)(y_0-x_0)\frac{(x_0-x)^\mu}{\mu!}\frac{(y-y_0)^\nu}{\nu!}$$

With this we get an approximation (3.1) where

$$\begin{aligned} \mathcal{I} &:= \mathbb{N}_0^d, \quad \mathcal{I}_m := \{(\mu,\nu)\in\mathcal{I}\times\mathcal{I} : |\mu+\nu| < m\}, \\ \kappa_{(\mu,\nu)}(x_0,y_0) &:= (D^{\mu+\nu}k)(y_0-x_0), \\ X_\mu(x;x_0) := \frac{(x_0-x)^\mu}{\mu!}, &\quad Y_\nu(y;y_0) := \frac{(y-y_0)^\nu}{\nu!}. \end{aligned} \tag{3.5}$$

The verification of the error bound (3.3) can be found in [14]. For example, (3.3) holds for the fundamental solution

$$k(x,y) \;=\; \frac{1}{4\pi|y-x|}, \quad x,y\in\mathbb{R}^3, x\neq y \tag{3.6}$$

of Laplace's equation in $\mathbb{R}^3$ with $C=1$ and $C(\eta) = -\log\eta$.

Remark 3.1. Note that only $\kappa_{(\mu,\nu)}$ depends on the kernel.

Applying the binomial formula the expansion (3.1) can be shifted from x_0 to x_1 and from y_0 to y_1 by

$$X_\mu(x;x_1) = \sum_{\substack{\nu\in\mathbb{N}_0^d\\ \nu\le\mu}} \frac{(x_1-x_0)^{\mu-\nu}}{(\mu-\nu)!}X_\nu(x;x_0) \qquad Y_\nu(y;y_1) = \sum_{\substack{\mu\in\mathbb{N}_0^d\\ \mu\le\nu}} \frac{(y_0-y_1)^{\nu-\mu}}{(\nu-\mu)!}Y_\mu(y;y_0) \tag{3.7}$$

3.1.2 Multipole Expansion [1]

The multipole expansion is the fastest and most specialized case of (3.1), i.e., the expansion coefficients must be evaluated analytically for each kernel of interest separately. Here we only present the multipole expansion for the Coulomb-potential in three dimensions [1].

The multipole expansion in $\mathbb{R}^3$ is given by an expansion of the kernel function (3.6) based on spherical harmonics:

$$Y_l^m(x) \;:=\; \sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}P_l^{|m|}(\cos\Theta)e^{im\phi}, \tag{3.8}$$

for $x\in\mathbb{S}_2$, $l\in\mathbb{N}_0$, $m\in\mathbb{Z}$, $|m|\le l$ and $(\Theta,\phi)\in[0,\pi]\times[0,2\pi)$ the spherical coordinates of x. The functions P_n^m are called associated Legendre functions and can be defined by the Rodrigues' formula

$$P_l^m(x) \;:=\; (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x), \qquad l,m\in\mathbb{N}_0, m\le l. \tag{3.9}$$

P_l denotes the Legendre polynomial

$$P_l(x) \;:=\; \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l, \qquad l\in\mathbb{N}_0. \tag{3.10}$$

Lemma 3.2. *Let $z, z_0 \in \mathbb{R}^3$ satisfying $|z-z_0| < |z_0|$. Then*

$$\frac{Y_l^m(\frac{z}{|z|})}{C_l^m|z|^{l+1}} \;=\; \sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} \frac{Y_{l+l'}^{m+m'}(\frac{z_0}{|z_0|})}{C_{l+l'}^{m+m'}|z_0|^{l+l'+1}}\, C_{l'}^{m'}|z_0-z|^{l'} Y_{l'}^{-m'}\Big(\frac{z_0-z}{|z_0-z|}\Big) \tag{3.11}$$

with C_l^m defined by

$$C_l^m \;=\; \frac{i^{|m|}}{\sqrt{(l-m)!(l+m)!}}. \tag{3.12}$$

For the proof see [1].

Applying Lemma 3.2 twice for given $x, y, x_0, y_0 \in \mathbb{R}^3$ with $|x-x_0|+|y-y_0| < |y_0-x_0|$ yields the multipole expansion of the Coulomb potential:

$$\begin{aligned} |y-x|^{-1} \;&=\; \frac{Y_0^0(\frac{y-x}{|y-x|})}{C_0^0|y-x|} = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^m|y_0-y|^l Y_l^{-m}(\frac{y_0-y}{|y_0-y|})\frac{Y_l^m(\frac{y_0-x}{|y_0-x|})}{C_l^m|y_0-x|^{l+1}} \\ &=\; \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'} C_l^m|y_0-y|^l Y_l^{-m}(\frac{y_0-y}{|y_0-y|}) \\ &\qquad \frac{Y_{l+l'}^{m+m'}(\frac{y_0-x_0}{|y_0-x_0|})C_{l'}^{m'}|x-x_0|^{l'}Y_{l'}^{-m'}(\frac{x-x_0}{|x-x_0|})}{C_{l+l'}^{m+m'}|y_0-x_0|^{l+l'+1}}. \end{aligned} \tag{3.13}$$

Truncating (3.13) we obtain an approximation (3.1) of the kernel with

$$\begin{aligned} &\mathcal{I} := \{\mu\in\mathbb{N}_0\times\mathbb{Z}:\ |\mu_2|\le\mu_1\}, \qquad \mathcal{I}_m := \{(\mu,\nu)\in\mathcal{I}\times\mathcal{I}:\ \mu_1+\nu_1<m\}, \\ &\kappa_{(\mu,\nu)}(x_0,y_0) := \frac{Y_{\mu_1+\nu_1}^{\mu_2+\nu_2}\Big(\dfrac{y_0-x_0}{|y_0-x_0|}\Big)}{C_{\mu_1+\nu_1}^{\mu_2+\nu_2}|y_0-x_0|^{\mu_1+\nu_1+1}}, \\ &X_\mu(x;x_0) := C_{\mu_1}^{\mu_2}|x-x_0|^{\mu_1}Y_{\mu_1}^{-\mu_2}\Big(\frac{x-x_0}{|x-x_0|}\Big), \qquad Y_\nu(y;y_0) := X_\nu(y_0;y). \end{aligned} \tag{3.14}$$

Moreover, this approximation satisfies the error bound (3.3) with $C(\eta)\sim 1/(1-\eta)$.

Lemma 3.3. *Let $z, z_0 \in \mathbb{R}^3$ satisfying $|z-z_0| < |z_0|$. Then*

$$Y_l^m\Big(\frac{z}{|z|}\Big)C_l^m|z|^l = \sum_{l'=0}^{l}\sum_{m'=-l'}^{l'} Y_{l-l'}^{m-m'}\Big(\frac{z-z_0}{|z-z_0|}\Big)C_{l-l'}^{m-m'}|z-z_0|^{l-l'}C_{l'}^{m'}|z_0|^{l'}Y_{l'}^{m'}\Big(\frac{z_0}{|z_0|}\Big) \tag{3.15}$$

with C_l^m defined as in Lemma 3.2.

The proof is the same as for Lemma 3.2 except using [1, Theorem 5.5] instead of [1, Theorem 5.3].

To reduce the number of operations to evaluate the approximation (3.14) we exploit

$$Y_l^{-m} = \overline{Y_l^m} \text{ and } \frac{i^{|m|}i^{|m'|}}{i^{|m+m'|}} = \begin{cases} 1 & \text{for } m', m \geq 0 \\ (-1)^{\min\{|m|,|m'|\}} & \text{otherwise} \end{cases} \tag{3.16}$$

and reformulate k_m by

$$\begin{aligned} k_m(x,y;x_0,y_0) &= \sum_{(\mu,\nu)\in\mathcal{I}_m} \mathcal{R}\Big(\kappa_{\mu+\nu}(x_0,y_0)X_\mu(x;x_0)Y_\nu(y;y_0)\Big) \\ &+ \sum_{\substack{(\mu,\nu)\in\mathcal{I}_m \\ 0<\mu_2\leq\nu_2}} (-1)^{\mu_2}\mathcal{R}\Big(\kappa_{(\nu_1+\mu_1,\nu_2-\mu_2)}(x_0,y_0)\overline{X_\mu(x;x_0)}Y_\nu(y;y_0)\Big) \\ &+ \sum_{\substack{(\mu,\nu)\in\mathcal{I}_m \\ 0<\nu_2\leq\mu_2}} (-1)^{\nu_2}\mathcal{R}\Big(\kappa_{(\mu_1+\nu_1,\mu_2-\nu_2)}(x_0,y_0)X_\mu(x;x_0)\overline{Y_\nu(y;y_0)}\Big) \end{aligned} \tag{3.17}$$

where $\mathcal{R}$ denotes the real part and obtain (3.1) with

$$\mathcal{I} := \{\mu \in \mathbb{N}_0 \times \mathbb{N}_0 : \ \mu_2 \leq \mu_1\}, \qquad \mathcal{I}_m := \{(\mu,\nu) \in \mathcal{I}\times\mathcal{I} : \ \mu_1+\nu_1 < m\},$$

$$\kappa_\mu(x_0,y_0) := 2^{1-\delta_{0\mu_2}}\frac{\sqrt{(\mu_1+\mu_2)!(\mu_1-\mu_2)!}}{|y_0-x_0|^{\mu_1+1}}Y_{\mu_1}^{\mu_2}\Big(\frac{y_0-x_0}{|y_0-x_0|}\Big),$$

$$X_\mu(x;x_0) := \frac{|x-x_0|^{\mu_1}}{\sqrt{(\mu_1+\mu_2)!(\mu_1-\mu_2)!}}Y_{\mu_1}^{-\mu_2}\Big(\frac{x-x_0}{|x-x_0|}\Big), \quad Y_\nu(y;y_0) := X_\nu(y_0;y).$$

3.1.3 Čebyšev Interpolation

The Taylor and multipole expansion coefficients have to be calculated for each kernel separately. To circumvent this we interpolate the kernel $k(x,y)$ by Čebyšev polynomials. For this only the kernel has to be evaluated at $O(m^d)$ different points and no derivatives come into play. Therefore it is easy to adapt the implementation to new kernels since only the evaluation routine of the kernel has to be replaced. We will verify Assumption 3.1 for this variant of clustering for general kernels with analytic far fields.

Let $I := [-1,1]$, $m \in \mathbb{N}_0$ and $T_\mu(x) = \cos(\mu \arccos(x))$, $\mu \in \mathbb{Z}$, denote the Čebyšev polynomials of the first kind. For any function f, defined on I, we consider the formal Čebyšev expansion

$$f(x) = \sum_{\mu\in\mathbb{Z}} \widehat{f}(\mu)T_\mu(x), \qquad \widehat{f}(\mu) := \frac{1}{\pi}\int_{-1}^{1}\frac{f(\xi)T_\mu(\xi)}{\sqrt{1-\xi^2}}d\xi \tag{3.18}$$

and the Čebyšev interpolant

$$f_m(x) := \sum_{\substack{\mu\in\mathbb{Z} \\ |\mu|<m}} \widehat{f}_\mu T_\mu(x), \qquad \widehat{f}_\mu := \frac{1}{m}\sum_{0\leq i<m} f(x_i)T_\mu(x_i) \tag{3.19}$$

where we assume f to be known at the m Čebyšev-points $x_i := \cos((i+1/2)\pi/m) \in I$, i.e., the m roots of T_m. By employing tensor products,

$$T_\mu(x) := \prod_{1\leq i\leq d} T_{\mu_i}((x)_i), \qquad \mu \in \mathbb{Z}^d, x \in I^d \tag{3.20}$$

we extend expansion and interpolation to the d-dimensional case with $(x)_i$ the i-th component of $x \in I^d$. This yields

$$f(x) = \sum_{\mu \in \mathbb{Z}^d} \widehat{f}(\mu) T_\mu(x), \qquad \widehat{f}(\mu) := \pi^{-d} \int_{I^d} \frac{f(\xi) T_\mu(\xi)}{\prod_{1 \le i \le d} \sqrt{1 - ((\xi)_i)^2}} d\xi \tag{3.21}$$

and

$$f_m(x) := \sum_{\substack{\mu \in \mathbb{Z}^d \\ |\mu|_\infty < m}} \widehat{f}_\mu T_\mu(x), \qquad \widehat{f}_\mu := m^{-d} \sum_{\substack{\nu \in \mathbb{N}_0^d \\ \nu_i < m}} f(x_\nu) T_\mu(x_\nu) \tag{3.22}$$

where $x_\nu := (x_{\nu_i})_{1 \le i \le d} \in I^d$ and $|\mu|_\infty = \max_{1 \le i \le d} |\mu_i|$.

Remark 3.4. Note that $T_{\mu_i}(x) = T_{-\mu_i}(x)$, $\sum_{\substack{\mu \in \mathbb{Z}^d \\ |\mu|_\infty < m}} \widehat{f}_\mu T_\mu(x) = \sum_{\substack{\mu \in \mathbb{N}_0^d \\ |\mu|_\infty < m}} 2^{d - |\delta_{\mu 0}|_1} \widehat{f}_\mu T_\mu(x)$ with $|\mu|_1 = \sum_{i=1}^d |\mu_i|$.

Lemma 3.5. *Suppose $f : I^d \to \mathbb{R}$ to be a continuous function that admits an Čebyšev expansion. Then interpolation* (3.22) *and expansion* (3.21) *are related by*

$$\widehat{f}_\mu = \sum_{\zeta \in \mathbb{Z}^d} (-1)^{|\zeta|_1} \widehat{f}(2m\zeta + \mu) \tag{3.23}$$

for all $\mu \in \mathbb{Z}^d$ with $|\mu|_\infty < m$. In particular, the Čebyšev interpolant of T_ν, $\nu \in \mathbb{Z}^d$, is given by $(-1)^{|\nu - \mu|_1/(2m)} T_\mu$ where $\mu \equiv \nu \bmod 2m$ and $|\mu|_\infty < m$.

Proof. Inserting the Čebyšev expansion of f in (3.22) we find

$$\begin{aligned} \widehat{f}_\mu &= m^{-d} \sum_{\substack{\iota \in \mathbb{N}_0^d \\ \iota_i < m}} \sum_{\nu \in \mathbb{Z}^d} \widehat{f}(\nu) T_\nu(x_\iota) T_\mu(x_\iota) = m^{-d} \sum_{\nu \in \mathbb{Z}^d} \widehat{f}(\nu) \sum_{\substack{\iota \in \mathbb{N}_0^d \\ \iota_i < m}} T_\nu(x_\iota) T_\mu(x_\iota) \\ &= m^{-d} \sum_{\nu \in \mathbb{Z}^d} \widehat{f}(\nu) \prod_{1 \le i \le d} \sum_{0 \le j < m} T_{\nu_i}(x_j) T_{\mu_i}(x_j). \end{aligned} \tag{3.24}$$

Since $2T_{\nu_i}(x) T_{\mu_i}(x) = T_{\nu_i + \mu_i}(x) + T_{\nu_i - \mu_i}(x)$ and

$$\sum_{0 \le j < m} T_{\mu_i}(x_j) = m \begin{cases} (-1)^{\frac{\mu_j}{2m}} & \text{if } \mu_i \equiv 0 \bmod 2m, \\ 0 & \text{otherwise} \end{cases}$$

the product in (3.24) does not vanish iff $\nu_i \equiv \pm \mu_i \bmod 2m$ for all $1 \le i \le d$. We restrict the summation to these values and exploit that $\widehat{f}(-\mu_i) = \widehat{f}(\mu_i)$. With this we get

$$\widehat{f}_\mu = \frac{1}{2} \sum_{\zeta \in \mathbb{Z}^d} \left((-1)^{|\zeta|_1} \widehat{f}(2m\zeta + \mu) + (-1)^{|\zeta|_1} \widehat{f}(2m\zeta - \mu) \right) = \sum_{\zeta \in \mathbb{Z}^d} (-1)^{|\zeta|_1} \widehat{f}(2m\zeta + \mu)$$

which yield the assertion. □

Lemma 3.6. *Let $\mathcal{E}_\rho \in \mathbb{C}$, $\rho > 1$, designate the closed ellipse with foci at ± 1 and sum of its semi-axis ρ. Suppose, $f : I^d \to \mathbb{R}$ admits an analytic extension into $\mathcal{E}_\rho^d := (\mathcal{E}_\rho)^d$. Then, for the Čebyšev interpolant* (3.22) *there holds the error estimate*

$$||f - f_m||_{L^\infty(I^d)} \;\leq\; \sqrt{d}\, 2^{\frac{d}{2}+1} \rho^{-m} (1-\rho^{-2})^{-\frac{d}{2}} M_\rho(f) \tag{3.25}$$

where $M_\rho(f) := \max_{z \in \mathcal{E}_\rho^d} |f(z)|$.

Proof. The verification of Lemma 3.6 consists in applying the generic error estimation technique of Davis for analytic functions [10, 25]. We introduce the inner product

$$(f,g)_\rho \;:=\; \int_{\mathcal{E}_\rho^d} \frac{f(z)\overline{g(z)}}{\prod_{1\leq i\leq d} \sqrt{|1-((z)_i)^2|}} dz \tag{3.26}$$

and consider the space

$$L^2(\mathcal{E}_\rho^d) \;:=\; \left\{ f : f \text{ analytic inside } \mathcal{E}_\rho^d \text{ and } \|f\|_\rho := \sqrt{(f,f)_\rho} < \infty \right\}.$$

Then, the polynomials

$$p_\mu(z) \;:=\; \left(\frac{2}{\pi}\right)^{\frac{d}{2}} \prod_{1\leq i\leq d} (\rho^{2\mu_i} + \rho^{-2\mu_i})^{-\frac{1}{2}} T_\mu(z), \qquad \mu \in \mathbb{N}_0^d \tag{3.27}$$

define a complete orthonormal set with respect to (3.26) such that for any bounded linear functional E over $L^2(\mathcal{E}_\rho^d)$ there holds

$$|E(f)|^2 \leq \|E\|_\rho^2 \|f\|_\rho^2 = \sum_{\mu\in\mathbb{N}_0^d} |E(p_\mu)|^2 \|f\|_\rho^2 = \|f\|_\rho^2 \sum_{\mu\in\mathbb{N}_0^d} |E(p_\mu)|^2 \tag{3.28}$$

for all $f \in L^2(\mathcal{E}_\rho^d)$. For $x \in I^d$ select E to be the error of interpolation in x, i.e.,

$$E(f) = E_x(f) := f(x) - f_m(x)\,. \tag{3.29}$$

This yields for the sum in (3.28)

$$\begin{aligned}
\sum_{\mu\in\mathbb{N}_0^d} |E_x(p_\mu)|^2 \;&=\; \left(\frac{2}{\pi}\right)^d \sum_{\mu\in\mathbb{N}_0^d} \prod_{1\leq i\leq d} (\rho^{2\mu_i} + \rho^{-2\mu_i})^{-1} |E_x(T_\mu)|^2 \\
&\leq\; 4\left(\frac{2}{\pi}\right)^d \sum_{\substack{\mu\in\mathbb{N}_0^d \\ |\mu|_\infty \geq m}} \prod_{1\leq i\leq d} (\rho^{2\mu_i} + \rho^{-2\mu_i})^{-1} \\
&\leq\; 4\left(\frac{2}{\pi}\right)^d \sum_{\substack{\mu\in\mathbb{N}_0^d \\ |\mu|_\infty \geq m}} \prod_{1\leq i\leq d} (\rho^{2\mu_i})^{-1} \leq 4d \left(\frac{2}{\pi}\right)^d \rho^{-2m} \sum_{\mu\in\mathbb{N}_0^d} \prod_{1\leq i\leq d} (\rho^{2\mu_i})^{-1} \\
&\leq\; 4d \left(\frac{2}{\pi}\right)^d \rho^{-2m} \sum_{\mu\in\mathbb{N}_0^d} \rho^{-2|\mu|_1} \leq 4d \left(\frac{2}{\pi}\right)^d \rho^{-2m} (1-\rho^{-2})^{-d},
\end{aligned} \tag{3.30}$$

since according to Lemma 3.5 $|E_x(T_\mu)| \leq 2$ for $|\mu|_\infty \geq m$ and obviously zero otherwise. Combining (3.30) and the bound $\|f\|_\rho^2 \leq \pi^d M_\rho(f)^2$ gives the assertion. □

Lemma 3.7. *Let $\rho > 1$, $r > 0$, $c \in \mathbb{R}^d$. Then $f : I^d \to \mathbb{R}$; $f(\xi) := |r\xi + c|^{-s}$, $s > 0$, can be extended analytically into $\mathcal{E}_\rho^d$ provided*

$$\frac{\|c\|_2}{r\sqrt{d}} \;>\; \sqrt{\frac{\rho^2+\rho^{-2}}{2}}. \tag{3.31}$$

In addition, suppose now $\rho = \|c\|_2/(r\sqrt{d})$, which satisfies (3.31)*, then the module of f on $\mathcal{E}_\rho^d$ is bounded by*

$$M_\rho(f) \;\le\; \left(\frac{(1-\rho^{-2})}{2}\sqrt{\frac{\rho^2-\rho^{-2}}{\rho^2+\rho^{-2}}}\right)^{-s} \|c\|_2^{-s}. \tag{3.32}$$

Proof. The extension of f given by

$$f(z) \;=\; \left(\sum_{i=1}^d (rz+c)_i^2\right)^{-\frac{s}{2}} \tag{3.33}$$

is analytic in $\Omega := \{z \in \mathbb{C}^d : \sum_{i=1}^d (rz+c)_i^2 \neq 0\}$. Writing $z_i \in \mathcal{E}_\rho$ as

$$z_i = \mathcal{R}(z_i) + \sqrt{-1}\mathcal{I}(z_i) = \frac{\rho+\rho^{-1}}{2}\cos(\phi_i) + \sqrt{-1}\frac{\rho-\rho^{-1}}{2}\sin(\phi_i) \qquad \phi_i \in [0,2\pi]$$

and using

$$\min_{\phi_i\in[0,2\pi]} a\cos(2\phi_i) + b\cos(\phi_i) \;\ge\; -a - \frac{b^2}{8a} \tag{3.34}$$

for $a \ge 0$ we find that for any $z \in \mathcal{E}_\rho^d$

$$\begin{aligned}
\mathcal{R}\Big(\sum_{i=1}^d (rz_i+c_i)^2\Big) &= \sum_{i=1}^d r^2(\mathcal{R}(z_i))^2 - r^2(\mathcal{I}(z_i))^2 + c_i^2 + 2r\mathcal{R}(z_i)c_i \\
&\ge \min_{\phi\in[0,2\pi]^d} \sum_{i=1}^d \frac{r^2}{4}(\rho^2+\rho^{-2})\cos(2\phi_i) + rc_i(\rho+\rho^{-1})\cos(\phi_i) + c_i^2 + \frac{r^2}{2} \\
&\ge \sum_{i=1}^d -\frac{r^2}{4}(\rho^2+\rho^{-2}) - \frac{(\rho+\rho^{-1})^2 c_i^2}{2(\rho^2+\rho^{-2})} + c_i^2 + \frac{r^2}{2} \\
&= \frac{(\rho-\rho^{-1})^2}{2}\sum_{i=1}^d \frac{c_i^2}{(\rho^2+\rho^{-2})} - \frac{r^2}{2} \ge \frac{(\rho-\rho^{-1})^2}{2}\Big(\frac{\|c\|_2^2}{(\rho^2+\rho^{-2})} - \frac{dr^2}{2}\Big) > 0
\end{aligned}$$

where we employ (3.31) to derive the last inequality. Hence, the real part of f does not vanish implying $\mathcal{E}_\rho^d \subset \Omega$. To estimate $M_\rho(f)$, note that

$$|f(z)| = \Big|\sum_{i=1}^d (rz+c)_i^2\Big|^{-\frac{s}{2}} \le \mathcal{R}\Big(\sum_{i=1}^d (rz+c)_i^2\Big)^{-\frac{s}{2}}.$$

In view of the estimation above the assertion follows. ∎

Theorem 3.2. *Let $0 < \eta < 1$, $s > 0$ and*

$$k : D \times D \to \mathbb{R}; \quad k(x,y) := K(y-x)|y-x|^{-s} \tag{3.35}$$

a kernel function where $D \subset \mathbb{R}^d$ and K admits an analytic extension into $\mathbb{C}^d \backslash \{0\}$. Suppose χ denotes for any $x_0, y_0 \in D$, $x_0 \neq y_0$, the affine transformation

$$\chi : \mathbb{R}^d \to \mathbb{R}^d; \quad \chi(\xi) := \eta ||y_0 - x_0||_\infty \xi + y_0 - x_0. \tag{3.36}$$

Then, the approximation of k given by the Čebyšev interpolant of $f(\cdot; x_0, y_0) := (K \circ \chi)|\chi|^{-s}$ on I^d,

$$k_m(x,y;x_0,y_0) := \sum_{\substack{\mu \in \mathbb{Z}^d \\ |\mu|_\infty < m}} \widehat{f}_\mu(x_0,y_0) T_\mu(\chi^{-1}(y-x)), \tag{3.37}$$

satisfies the error bound (3.3)*. In addition, k_m admits the representation* (3.1) *with*

$$\begin{aligned} \mathcal{I}_m &:= \{(\mu,\nu) \in \mathbb{N}_0^d \times \mathbb{N}_0^d : \, |\mu+\nu|_\infty < m\}, \\ \kappa_{(\mu,\nu)}(x_0,y_0) &:= (\mu+\nu)! c_{\mu+\nu}(x_0,y_0), \\ X_\mu(x,x_0) := \frac{(x_0-x)^\mu}{\mu!}, &\qquad Y_\nu(y,y_0) := \frac{(y-y_0)^\nu}{\nu!}. \end{aligned} \tag{3.38}$$

where the c_μ, $\mu \in \mathbb{N}_0^d$, are the coefficients of the interpolation polynomial defined by

$$\sum_{\substack{\mu \in \mathbb{Z}^d \\ |\mu|_\infty < m}} \widehat{f}_\mu(x_0,y_0) T_\mu\Big(\frac{z}{\eta ||y_0 - x_0||_\infty}\Big) = \sum_{\substack{\mu \in \mathbb{N}_0^d \\ |\mu|_\infty < m}} c_\mu(x_0,y_0) z^\mu. \tag{3.39}$$

To get (3.38) we interpolate the kernel function by Čebyšev polynomials

$$k_m(x,y;x_0,y_0) = \sum_{\substack{\mu \in \mathbb{Z}^d \\ |\mu| < m}} \widehat{f}_\mu(x_0,y_0) T_\mu(\chi^{-1}(y-x)) \tag{3.40}$$

where the m^d expansion coefficients are given by

$$\widehat{f}_\mu(x_0,y_0) = m^{-d} \sum_{\substack{\nu \in \mathbb{N}_0^d \\ \nu_i < m}} (K \circ \chi)(x_\nu) |\chi(x_\nu)|^{-s} T_\mu(x_\nu) \tag{3.41}$$

Expanding the interpolant by Taylor we get

$$\begin{aligned} k_m(x,y;x_0,y_0) &= \sum_{\substack{\zeta \in \mathbb{Z}^d \\ |\zeta|_\infty < m}} \widehat{f}_\zeta(x_0,y_0) T_\zeta(\chi^{-1}(y-x)) \\ &= \sum_{\substack{\zeta \in \mathbb{Z}^d \\ |\zeta|_\infty < m}} \widehat{f}_\zeta(x_0,y_0) T_\zeta\left(\frac{y-x-y_0+x_0}{\eta ||y_0-x_0||_\infty}\right) = \sum_{\substack{\zeta \in \mathbb{N}_0^d \\ |\zeta|_\infty < m}} c_\zeta(x_0,y_0)(y-x-y_0+x_0)^\zeta \\ &= \sum_{(\nu,\mu) \in \mathbb{N}_0^d \times \mathbb{N}_0^d} \sum_{\substack{\zeta \in \mathbb{N}_0^d \\ |\zeta|_\infty < m}} c_\zeta(x_0,y_0) D^{\mu+\nu}(z^\zeta)(0) \frac{(x_0-x)^\mu}{\mu!} \frac{(y-y_0)^\nu}{\nu!} \\ &= \sum_{\substack{(\nu,\mu) \in \mathbb{N}_0^d \times \mathbb{N}_0^d \\ |\mu+\nu|_\infty < m}} \frac{(x_0-x)^\mu}{\mu!} \frac{(y-y_0)^\nu}{\nu!} (\mu+\nu)! c_{\mu+\nu}(x_0,y_0). \end{aligned}$$

Remark 3.8. There is only an error in the interpolation. Taylor expansion is exact since the derivatives of order larger than m of a polynomial of degree m vanish.

Remark 3.9. The coefficients $\widehat{f}_\mu(x_0, y_0)$ in (3.39) - (3.41) require $O(m^d)$ kernel evaluations at the Čebyšev points of order m. The kernel is not explicitly needed, but could for example be given in a subroutine.

3.1.4 Fast Helmholtz Solvers

In acoustics and electromagnetics, the kernel function

$$k(x, y) = \frac{e^{i\lambda|x-y|}}{4\pi|x-y|} \tag{3.42}$$

arises. It is an easy exercise to verify that Čebyšev-Interpolation can be applied, since $k(x, y)$ satisfies the assumptions of Theorem 3.2. However, for high wavenumber λ in (3.42), polynomial farfield interpolation is inefficient, i.e. very high expansion order m is needed for an efficient scheme. In [8] and the references there, the approximation

$$k_m(x, y) = \sum_p \omega_p \, e^{i\lambda\langle s_p, x-x_0\rangle} \, T_\ell(x_0 - y_0; s_p) e^{i\lambda\langle s_p, y_0-y\rangle} \tag{3.43}$$

is introduced. Here, ω_p and s_p are weights and nodes of a quadrature formula on the sphere, i.e.

$$\int_{S^2} f(x) \sim \sum_p \omega_p \, f(s_p) \,,$$

and $T_\ell(x_0 - y_0; s_p)$ denotes a transfer operator (see [8] for details).

Once again, (3.43) is of the form (3.1) with $\mu = (\ell, p)$, $\nu = (\ell, p)$ and

$$X_\mu(x, x_0) = e^{i\lambda\langle s_p, x-x_0\rangle}, \; Y_\nu(y; y_0) = e^{-i\lambda\langle s_p, y-y_0\rangle}$$

$$\kappa_{(\mu,\nu)}(x_0, y_0) = \omega_p \, T_\ell(x_0 - y_0; s_p) \,.$$

The validity of the error bound (3.3) has been established in [9].

3.2 Cluster Expansions

Assumption 3.1 provides an approximation of the kernel, which is in general not valid for all $(x, y) \in \Gamma \times \Gamma$. In order to define a global approximation on $\Gamma \times \Gamma$, a collection of local approximations is used, where each of the local approximation is associated with an appropriate block of a given partition of $\Gamma \times \Gamma$. Those blocks are called *clusters* and the combination of local approximations a *cluster expansion*.

More precisely, let $\mathcal{P}(\Gamma)$ denote the set of all subsets of Γ, $\check{r}_A := \inf_{x\in\mathbb{R}^d} \sup_{y\in A} |y - x| \in \mathbb{R}$ the Čebyšev radius of a set $A \subset \mathbb{R}^d$ and $\check{c}_A \in \mathbb{R}^d$ with $\check{r}_A = \sup_{y\in A} |y - \check{c}_A|$ its Čebyšev center.

Definition 3.10. *Suppose $\mathcal{C} \subset \mathcal{P}(\Gamma) \times \mathcal{P}(\Gamma)$ to be a finite partition of $\Gamma \times \Gamma$ and let $0 < \eta < 1$. An element $(\sigma, \tau) \in \mathcal{C}$ is called η-cluster iff*

$$\check{r}_\sigma + \check{r}_\tau \quad \leq \quad \eta \left| \check{c}_\sigma - \check{c}_\tau \right| . \tag{3.44}$$

The set of all η-clusters in $\mathcal{C}$,

$$\mathcal{F} := \mathcal{F}(\mathcal{C}, \eta) = \{(\sigma, \tau) \in \mathcal{C} : \ (\sigma, \tau) \ \textit{is } \eta\textit{-cluster}\} , \tag{3.45}$$

is called the far field of grain η and its complement $\mathcal{N} := \mathcal{N}(\mathcal{C}, \eta) = \mathcal{C} \setminus \mathcal{F}(\mathcal{C}, \eta)$ the associated near field. Moreover, let the kernel $k(x, y)$ satisfy Assumption 3.1. Then

$$k_m(x, y) := \begin{cases} k_m(x, y; \check{c}_\sigma, \check{c}_\tau) & \textit{if } (x, y) \in \sigma \times \tau \textit{ and } (\sigma, \tau) \in \mathcal{F} \\ k(x, y) & \textit{otherwise} \end{cases} \tag{3.46}$$

for all $(x, y) \in \Gamma \times \Gamma$, $x \neq y$, defines a cluster expansion of the kernel $k(x, y)$.

Proposition 3.11. *By construction, the local error bound (3.3) remains valid for a cluster expansion:*

$$|k(x, y) - k_m(x, y)| \leq C_0 (C_1 \eta)^m \, |k(x, y)| \tag{3.47}$$

for all $(x, y) \in \Gamma \times \Gamma$, $x \neq y$.

Replacing the kernel $k(x, y)$ in the definition of the system matrix $\boldsymbol{A}^L$ in (2.18) introduces an approximation $\widetilde{\boldsymbol{A}}^L$:

$$(\widetilde{\boldsymbol{A}}^L)_{ij} = \int_\Gamma \int_\Gamma k_m(x, y) \, \varphi_i^L(x) \, \varphi_j^L(y) \, ds_y \, ds_x \, .$$

Due to the properties of the cluster expansion, $\widetilde{\boldsymbol{A}}^L$ may be decomposed in the following way:

$$\widetilde{\boldsymbol{A}}^L = \boldsymbol{N}^L + \sum_{(\sigma,\tau) \in \mathcal{F}} {\boldsymbol{X}_\sigma^L}^T \boldsymbol{F}_{\sigma\tau} \boldsymbol{Y}_\tau^L \tag{3.48}$$

with

$$(\boldsymbol{N}^L)_{i,j} \ := \ \sum_{(\sigma,\tau) \in \mathcal{N}} \int_\sigma \int_\tau k(x, y) \varphi_i^L(x) \, \varphi_j^L(y) \, ds_y \, ds_x \, , \tag{3.49}$$

$$(\boldsymbol{X}_\sigma^L)_{\mu,i} \ := \ \int_\sigma X_\mu(x; \check{c}_\sigma) \varphi_i^L(x) \, ds_x, \tag{3.50}$$

$$(\boldsymbol{Y}_\tau^L)_{\nu,j} \ := \ \int_\tau Y_\nu(y; \check{c}_\tau) \varphi_j^L(y) \, ds_y \tag{3.51}$$

$$(\boldsymbol{F}_{\sigma\tau})_{\mu,\nu} \ := \ \kappa_{(\mu,\nu)}(\check{c}_\sigma, \check{c}_\tau) \tag{3.52}$$

for $(\sigma, \tau) \in \mathcal{F}$ and $(\mu, \nu) \in \mathcal{I}_m$. The matrix $\boldsymbol{N}^L$ represents the near field part of $\widetilde{\boldsymbol{A}}^L$ whereas the sum of matrices describes the influence of the far field. If the partition $\mathcal{C}$ is chosen as discussed in the next Section, $\boldsymbol{N}^L$ is a sparse matrix. In addition, the matrix vector multiplication related to the far field part can be evaluated with essentially linear complexity.

Remark 3.12. The matrices $\boldsymbol{F}_{\sigma\tau}$ are never formed explicitly. Typically, their entries $(\boldsymbol{F}_{\sigma\tau})_{\mu\nu}$ only depend on $\mu+\nu$ with $|\nu+\mu| < m$. Therefore, only $O(m^p)$ instead of $O(m^{2p})$ enties, where $p \in \{2,3\}$ is given by the chosen kernel expansion, have to be evaluated and stored. In order to form matrix vector products several algorithms to shift the expansion centers exist in the literature, which exploit features specific to the chosen expansion to reduce the $O(m^{2p})$ complexity of a standard matrix vector product. The various shift methods might be grouped into exact methods [15][12] and sparse approximations [8] which introduce an additional error, e.g. due to quadratures over S^2. The present paper only realizes the exact algorithms.

Remark 3.13. Derivatives of $D_x^\alpha D_y^\beta k(x,y)$ are easily handled by applying the derivatives to the kernel expansion. This way, only the matrices $\boldsymbol{X}_\sigma^L$ and $\boldsymbol{Y}_\tau^L$, respectively, have to be modified.

Remark 3.14. The kernel expansions listed in the previous Section preserve the symmetry of the kernel k, i.e. $k_m(x,y) = k_m(y,x)$. If, in addition, the given partition $\mathcal{C}$ exhibits symmetry, i.e. $(\sigma,\tau) \in \mathcal{C} \Rightarrow (\tau,\sigma) \in \mathcal{C}$, then $\widetilde{\boldsymbol{A}}^L$ is symmetric for Galerkin discretizations.

3.3 Cluster Algorithm

Equation (3.48) specifies an approximation of the system matrix $\boldsymbol{A}^L$ which allows to control the approximation error (see Section 3.4). However, the objective is, to reduce the complexity of assembly and storage of $\boldsymbol{A}^L$, which is closely related to the question of choosing the partition $\mathcal{C}$ appropriately. An efficient way, which also provides the desired complexity reduction, is to start with a recursive hierarchical decomposition of the mesh $\mathcal{M}^L$ represented by a tree $\mathcal{T} := (\mathcal{V},\mathcal{E})$. An algorithm similar to Algorithm 3.1 might be used to generate such a decomposition, i.e. $\mathcal{T} := \text{tree}(\mathcal{M}^L)$.

Algorithm 3.1 $(\mathcal{V},\mathcal{E}) := \text{tree}(A)$

---

if $|A| < c$ then
  return $(\{A\},\emptyset)$;
else
  $(A_0,A_1) := \text{split}(A)$
  $(\mathcal{V}_0,\mathcal{E}_0) := \text{tree}(A_0)$; $(\mathcal{V}_1,\mathcal{E}_1) := \text{tree}(A_1)$;
  return $(\mathcal{V}_0 \cup \mathcal{V}_1 \cup \{A\},\ \mathcal{E}_0 \cup \mathcal{E}_1 \cup \{(A,A_0),(A,A_1)\})$;

The function split(A) bisects a set of panels A into two disjoint sets A_0 and A_1 such that the Čebyšev radius of both sets is reduced. This, for example, could be achieved by splitting the bounding box of A along the longest side and distribute the panels with respect to the two parts.

Given a hierarchical decomposition $\mathcal{T}$ of $\mathcal{M}^L$ it is straight forward to construct a partition $\mathcal{C}$ as outlined in Algorithm 3.2. The decomposition $\mathcal{T}$ serves two purposes during the construction process: (i) it defines the pool $\mathcal{V}$ of subsets available for the construction of clusters and (ii) it defines the sets children$(A) := \{A' \in \mathcal{V} : \exists (A,A') \in \mathcal{E}\}$. Calling partition$(\mathcal{M}^L,\mathcal{M}^L)$ generates a partition $\mathcal{C}$ by specifying its far field $\mathcal{F}$ and near field $\mathcal{N}$. The generated partition is symmetric in the sense of Remark 3.14.

Note that in Algorithm 3.2 $\mathcal{N}$ and $\mathcal{F}$ are given in terms of sets of panels instead of subsets of the boundary Γ (cf. Definition 3.10).

Algorithm 3.2 $(\mathcal{N}, \mathcal{F}) := \text{partition}(A, B)$

if $(\bigcup_{\pi\in A}\pi, \bigcup_{\pi\in B}\pi)$ is an η-cluster then
  return $(\emptyset, \{(A, B)\})$;
else
  $A' := \text{children}(A)$; $B' := \text{children}(B)$;

$$\text{return} \begin{cases} \bigcup_{a\in A', b\in B'} \text{partition}(a, b) & \text{if } A' \neq \emptyset \text{ and } B' \neq \emptyset \text{ and } |A| = |B|, \\ \bigcup_{a\in A'} \text{partition}(a, B) & \text{if } A' \neq \emptyset \text{ and } (|A| > |B| \text{ or } B' = \emptyset), \\ \bigcup_{b\in B'} \text{partition}(A, b) & \text{if } (|A| < |B| \text{ or } A' = \emptyset) \text{ and } B' \neq \emptyset, \\ (\{(A, B)\}, \emptyset) & \text{otherwise;} \end{cases}$$

The matrix vector product $\underline{v} = \widetilde{\boldsymbol{A}}^L \underline{u}$ is evaluated in five steps:

(i) compute $\underline{v}_{\mathcal{N}} := \boldsymbol{N}^L \underline{u}$,
(ii) for all τ compute $\underline{u}_\tau := \boldsymbol{Y}_\tau^L \underline{u}$,
(iii) for all σ compute $\underline{v}_\sigma := \sum_{(\sigma,\tau)\in\mathcal{F}} \boldsymbol{F}_{\sigma\tau} \underline{u}_\tau$,
(iv) compute $\underline{v}_{\mathcal{F}} := \sum_\sigma \boldsymbol{X}_\sigma^{L\,T} \underline{v}_\sigma$,
(v) compute $\underline{v} = \underline{v}_{\mathcal{N}} + \underline{v}_{\mathcal{F}}$.

The steps (ii) and (iv) can be accelerated taking once again advantage of the hierarchical decomposition. For most of the common kernel expansions it is possible to represent the matrices $\boldsymbol{X}_\sigma^L$ and $\boldsymbol{Y}_\tau^L$ by means of the corresponding matrices related to children of σ and τ:

$$\boldsymbol{X}_\sigma^L = \sum_{\sigma'\in\text{children}(\sigma)} \boldsymbol{C}_{\sigma\sigma'} \boldsymbol{X}_{\sigma'}^L, \qquad \boldsymbol{Y}_\tau^L = \sum_{\tau'\in\text{children}(\tau)} \boldsymbol{D}_{\tau\tau'} \boldsymbol{Y}_{\tau'}^L, \tag{3.53}$$

where the matrices $C_{\sigma\sigma'}$ and $D_{\tau\tau'}$ represent so-called shift operators (e.g. see Lemma 3.3 and (3.7)). These relationships are exploited in Algorithm 3.3 and 3.4, which replace step (ii) and (iv) above, i.e. by scatter$(\mathcal{M}^L, u)$ and $\underline{v}_{\mathcal{F}} := \text{gather}(\mathcal{M}^L, 0)$. Note that only the matrices $\boldsymbol{Y}_\tau^L$ and $\boldsymbol{X}_\sigma^L$, where τ and σ are leafs of the decomposition, are necessary. These matrices typically contain only $O(m^p)$ entries (see Remark 3.12).

Algorithm 3.3 scatter$(A, \underline{u})$

$\tau := \bigcup_{\pi\in A}\pi$; $A' := \text{children}(A)$;
if $A' = \emptyset$ then
  $\underline{u}_\tau := \boldsymbol{Y}_\tau^L u$;
else
  $\underline{u}_\tau := \sum_{a\in A'} \boldsymbol{D}_{\tau\tau'} \text{scatter}(a, \underline{u})$ with $\tau' := \bigcup_{\pi\in a}\pi$;
return $\underline{u}_\tau$;

Remark 3.15. Variations of the above algorithms include shift operators which are approximations. They are used, for example, to provide information on higher levels which is not explicitly available on lower levels of the decomposition [28] or simply to speed up the evaluation process [8].

Algorithm 3.4 gather$(A, \underline{w}_A)$

$\sigma := \bigcup_{\pi \in A} \pi$; $\quad A' := \text{children}(A)$;
if $A' = \emptyset$ then
  return ${\boldsymbol{X}_\sigma^L}^T(\underline{v}_\sigma + \underline{w}_A)$;
else
  return $\sum_{a \in A'} \text{gather}(a, {\boldsymbol{C}_{\sigma\sigma'}}^T(\underline{v}_\sigma + \underline{w}_A))$ with $\sigma' := \bigcup_{\pi \in a} \pi$;

3.4 Cluster error

The replacement (3.1) of $k(x,y)$ by the cluster approximation k_m in the far field introduces an approximate bilinear form via

$$\widetilde{a}(u^L, v^L) = \int_\Gamma \int_\Gamma \overline{v^L(x)}\, k_m(x,y)\, u^L(y) ds_y\, ds_x \tag{3.54}$$

where $k_m(x,y)$ is the global cluster expansion of the kernel $k(x,y)$ introduced in (3.46) and where $u^L, v^L \in V^L$. We can associate the form $\widetilde{a}(\cdot,\cdot)$ with the matrix $\widetilde{\boldsymbol{A}}^L$ and an approximate boundary element solution $\widetilde{\sigma}^L \in V^L$ via the perturbed variational problem:

$$\widetilde{\sigma}^L \in V^L : \ \widetilde{a}(\widetilde{\sigma}^L, v^L) = \langle \widetilde{f}, v^L \rangle \quad \forall v^L \in V^L . \tag{3.55}$$

We assume for now that we have an exact solution $\underline{\widetilde{\sigma}}^L$ of the perturbed linear system (incomplete iterative solution of (3.55) will be dealt with below)

$$\widetilde{\boldsymbol{A}}^L \underline{\widetilde{\sigma}}^L = \underline{\widetilde{f}}^L . \tag{3.56}$$

Our purpose is to estimate the error $\|\sigma - \widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma}$. The following Strang-type Lemma relates this error to the errors $a(\cdot,\cdot) - \widetilde{a}(\cdot,\cdot)$ and $f - \widetilde{f}$. We start by establishing the stability of (3.55).

Proposition 3.16. *Assume* (2.12), (2.13) *and that the bilinear form* $\widetilde{a}(\cdot,\cdot)$ *is consistent with* $a(\cdot,\cdot)$ *in the following sense: for every* $\delta > 0$ *there exists* $L_0(\delta)$ *such that for every* $L \geq L_0$,

$$|a(u^L, v^L) - \widetilde{a}(u^L, v^L)| \leq \delta \, \|u^L\|_{-\frac{1}{2},\Gamma} \, \|v^L\|_{-\frac{1}{2},\Gamma} \quad \forall u^L, v^L \in V^L . \tag{3.57}$$

Then the perturbed Galerkin scheme (3.55) *is stable, i.e. there are* $\gamma > 0$, $L_0 > 0$ *such that for all* $L \geq L_0$ *holds*

$$\forall u^L \in V^L : \sup_{v^L \in V^L} \frac{|\widetilde{a}(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \geq \gamma \|u^L\|_{-\frac{1}{2},\Gamma} \tag{3.58}$$

and

$$\forall v^L \in V^L : \sup_{u^L \in V^L} \frac{|\widetilde{a}(u^L, v^L)|}{\|u^L\|_{-\frac{1}{2},\Gamma}} \geq \gamma \|v^L\|_{-\frac{1}{2},\Gamma} . \tag{3.59}$$

Proof. (2.12) and (2.13) imply (2.19). We show (3.58). Given $0 \neq u^L \in V^L$, (2.19) and (3.57) give

$$\begin{aligned}\sup_{v^L \in V^L} \frac{|\widetilde{a}(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} &\geq \sup_{v^L \in V^L} \left\{ \frac{|a(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} - \frac{|a(u^L, v^L) - \widetilde{a}(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \right\} \\ &\geq \gamma \|u^L\|_{-\frac{1}{2},\Gamma} - \sup_{v^L \in V^L} \frac{|a(u^L, v^L) - \widetilde{a}(u^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \geq (\gamma - \delta) \|u^L\|_{-\frac{1}{2},\Gamma}.\end{aligned}$$

Choosing in (3.57) $\delta = \gamma/2$ and possibly adjusting L_0 yields (3.58). The proof of (3.59) is analogous. □

We obtain from (3.58), (3.59) that for sufficiently large L the problem (3.55) is well-posed. In particular, the matrix $\widetilde{\boldsymbol{A}}^L$ is nonsingular and the approximate solution $\widetilde{\sigma}^L \in V^L$ is well-defined. We derive now an error estimate for $\sigma - \widetilde{\sigma}^L$.

Proposition 3.17. *Assume* (3.57) *and that* $L \geq L_0$, L_0 *sufficiently large. Then the perturbed Galerkin solutions* $\widetilde{\sigma}^L$ *of* (3.55) *exist and satisfy the error estimate*

$$\|\sigma - \widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma} \leq C \left\{ \inf_{v^L \in V^L} \|\sigma - v^L\|_{-\frac{1}{2},\Gamma} + \delta \|f\|_{\frac{1}{2},\Gamma} + \sup_{v^L \in V^L} \frac{|\langle f - \widetilde{f}, v^L \rangle|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \right\} \tag{3.60}$$

where $C > 0$ *is independent of* $L \geq L_0$ *and* δ *as in* (3.57).

Proof. For $\delta > 0$ sufficiently small and $L \geq L_0(\delta)$, (3.58) gives

$$\begin{aligned}\|\sigma - \widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma} &\leq \|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} + \|\sigma^L - \widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma} \\ &\leq \|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} + \frac{1}{\gamma} \sup_{v^L \in V^L} \frac{|\widetilde{a}(\sigma^L - \widetilde{\sigma}^L, v^L)|}{\|v^L\|_{-\frac{1}{2},\Gamma}} \\ &= \|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} + \frac{1}{\gamma} \sup_{v^L \in V^L} \frac{1}{\|v^L\|_{-\frac{1}{2},\Gamma}} |\widetilde{a}(\sigma^L, v^L) - \langle \widetilde{f}, v^L \rangle| \\ &\leq \|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} + \frac{1}{\gamma} \sup_{v^L \in V^L} \frac{1}{\|v^L\|_{-\frac{1}{2},\Gamma}} \left\{ |\widetilde{a}(\sigma^L, v^L) - a(\sigma^L, v^L)| + |\langle f - \widetilde{f}, v^L \rangle| \right\}.\end{aligned}$$

Now (3.57) gives

$$\|\sigma - \widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma} \leq \|\sigma - \sigma^L\|_{-\frac{1}{2},\Gamma} + \frac{\delta}{\gamma} \|\sigma^L\|_{-\frac{1}{2},\Gamma} + \sup_{v^L \in V^L} \frac{|\langle f - \widetilde{f}, v^L \rangle|}{\|v^L\|_{-\frac{1}{2},\Gamma}}.$$

The stability (2.21) and the quasi optimality (2.20) of the Galerkin solution σ^L imply (3.60). □

We now link the discretization error $\sigma - \sigma^L$ and the consistency error $\sigma^L - \widetilde{\sigma}^L$ caused by the cluster approximation k_m in (3.46) of the kernel $k(x, y)$.

Theorem 3.18. *Assume* (2.12), (2.13) *and let a cluster approximation* k_m *of the far field be given which satisfies Assumption* 3.1 *with sufficiently small grain* η*. Choose the expansion order* m *according to*

$$m \geq CL \;\text{ or }\; m \geq C\,|\log h|\,, \tag{3.61}$$

with $C > 0$ *sufficiently large. Then*

i) there is $L_0 > 0$ *such that the Galerkin discretization* (3.55) *with clustering is stable and*

ii) the Galerkin solution $\widetilde{\sigma}^L$ *in* (3.55) *with* $\widetilde{f} = f$ *converges at the same rate as* σ^L*, i.e.*

$$\|\sigma - \widetilde{\sigma}^L\|_{H^{-\frac{1}{2}}(\Gamma)} \leq C h_L^{\min(s,\frac{3}{2})} \|f\|_{H^{\frac{1}{2}+s}(\Gamma)},\; L \geq L_0\,. \tag{3.62}$$

Proof. We show that the form $a(\cdot,\cdot)$ in (3.54) satisfies (3.57). We have

$$|a(u^L, v^L) - \widetilde{a}(u^L, v^L)| = \Big| \int\limits_{x\in\Gamma} \int\limits_{y\in\Gamma} \overline{v^L(x)}(k(x,y) - k_m(x,y))\, u^L(y)\, ds_y\, ds_x \Big|\,. \tag{3.63}$$

Since $v^L \in V^L = \mathrm{span}\{\varphi_i^L\}$, $\varphi_i^L = |\pi_i^L|^{-\frac{1}{2}}\,\chi_{\pi_i^L}$, $\pi_i^L \in \mathcal{M}^L$, we write $u^L = \sum_{\pi_i^L} u_i^L\,\varphi_i^L$, $v^L = \sum_{\pi_j^L} u_j^L\,\varphi_j^L$ and we have due to $\langle \varphi_i^L, \varphi_j^L\rangle = \delta_{ij}$ the norm equivalences

$$\|u^L\|_{0,\Gamma}^2 = \sum_i |u_i^L|^2 = \|\underline{u}^L\|_{\ell_2}^2,\; \|v^L\|_{0,\Gamma}^2 = \sum_j |v_j^L|^2 = \|\underline{v}^L\|_{\ell_2}^2\,.$$

Since the mesh $\mathcal{M}^L$ is shape-regular, there holds the inverse inequality with $h_{\min}$ denoting the smallest element diameter of $\mathcal{M}^L$

$$\forall u^L \in V^L:\; c_1 \|u^L\|_{-\frac{1}{2},\Gamma} \leq \|u^L\|_{L^2(\Gamma)} \leq c_2\, h_{\min}^{-\frac{1}{2}} \|u^L\|_{-\frac{1}{2},\Gamma} \tag{3.64}$$

where c_1, c_2 depend only on the shape regularity of $\mathcal{M}^L$. We can therefore estimate (3.63) as follows:

$$\Big| \int\limits_{\Gamma} \int\limits_{\Gamma} \overline{v^L(x)}\,\big(k(x,y) - k_m(x,y)\big)\, u^L(x)\, ds_y\, ds_x \Big| \leq \sum_{i,j} |\overline{v_i^L}\, E_{ij}^L\, u_j^L|$$

where

$$E_{ij}^L := \int\limits_{\pi_i^L} \int\limits_{\pi_j^L} |k(x,y) - k_m(x,y)|\, \varphi_i^L(x)\, \varphi_j^L(y)\, ds_y\, ds_x\,. \tag{3.65}$$

By Definition 3.10, $E_{ij}^L = 0$ if π_j^L is in the near field of π_i^L and vice versa (i.e. all singular integrals in $\widetilde{\boldsymbol{A}}^L$ are calculated exactly) and $E_{i,j}^L \neq 0 \Longrightarrow \mathrm{dist}(\pi_i^L, \pi_j^L) \geq c h_L$ for some $c > 1$ independent of L. Since φ_i^L is piecewise constant on $\mathcal{M}^L = \{\pi_i^L\}$, it follows with (3.47) that for $\mathrm{dist}(\pi_i^L, \pi_j^L) > c h_L$

$$\begin{aligned} |E_{ij}^L| &\leq h_L^{-2} \int\limits_{\pi_i^L} \int\limits_{\pi_j^L} |k(x,y) - k_m(x,y)|\, ds_y\, ds_x \leq h_L^2 \max_{x\in\pi_i^L} \max_{y\in\pi_j^L} \big\{|k(x,y) - k_m(x,y)|\big\} \\ &\leq h_L^2\, C_0 (C_1\eta)^m \max_{x\in\pi_i^L} \max_{y\in\pi_j^L} |k(x,y)| \leq C h_L^2\, C_0 (C_1\eta)^m \big(\mathrm{dist}(\pi_i^L, \pi_j^L)\big)^{-\widetilde{s}} \end{aligned}$$

where $\widetilde{s}=1$ denotes the singularity order. Hence we get $\forall u^L, v^L \in V^L$:

$$|\widetilde{a}(u^L,v^L)-a(u^L,v^L)| = C\sum_{i,j} u_i^L\, v_j^L\, h_L^2\, C_0(C_1\eta)^m\ \ d_{ij}^{-\widetilde{s}}$$

where $d_{ij}=\mathrm{dist}(\pi_i^L,\pi_j^L)$. Using the Cauchy-Schwarz inequality, we get

$$\begin{aligned}|a(u^L,v^L)-\widetilde{a}(u^L,v^L)| &\le C\,C_0(C_1\eta)^m(\min_{ij} d_{ij})^{-\widetilde{s}}\, h_L^2\Big(\sum_i |u_i^L|^2\Big)^{\frac12}\Big(\sum_j |v_j^L|^2\Big)^{\frac12}\\ &\le C\,C_0(C_1\eta)^m\, h_L^{-\widetilde{s}+2}\,\|u^L\|_{0,\Gamma}\,\|v^L\|_{0,\Gamma}\,,\end{aligned}$$

and using (3.64)

$$|a(u^L,v^L)-\widetilde{a}(u^L,v^L)| \le C\,C_0(C_1\eta)^m h_L^{-\widetilde{s}+1}\,\|u^L\|_{-\frac12,\Gamma}\|v^L\|_{-\frac12,\Gamma}\,. \tag{3.66}$$

With $\widetilde{s}=1$ we get from (3.66) that (3.57) holds with $\delta = C\,C_0(C_1\eta)^m$. We choose $\eta>0$ so small that $C_1\eta<1/2$ and obtain $\delta<h_L^{\frac32}$ if $m>C\,|\log h_L| = CL$ for a sufficiently large C, i.e. if (3.61) holds. This also implies that $\delta\to 0$, as $L\to\infty$. Therefore, Proposition 3.17 applies and $\widetilde{a}(\cdot,\cdot)$ is stable for sufficiently large L. Since $\widetilde{f}=f$ was assumed, (3.60) implies that

$$\|\sigma-\widetilde{\sigma}^L\|_{-\frac12,\Gamma} \le C\Big\{\inf_{v^L\in V^L}\|\sigma-v^L\|_{-\frac12,\Gamma}+h^{\frac32}\,\|f\|_{\frac12,\Gamma}\Big\}.$$

The assertion (3.62) follows from the approximation property (2.23) of V^L and the $H^{-\frac12+s}(\Gamma)$ regularity of σ. □

Remark 3.19. In the proof of Theorem 3.18, we assumed $\widetilde{s}=1$, corresponding to the weakly singular operator V. The same analysis, however, also applies to a cluster approximation $\widetilde{b}(\cdot,\cdot)$ of the form $b(\cdot,\cdot)$ in the right hand side of the direct Galerkin BEM (2.28). We use then $\widetilde{s}=0$ and Proposition 3.17 with

$$|\langle f-\widetilde{f},v^L\rangle| = |b(f,v^L)-\widetilde{b}(f,v^L)| \le Ch_L^{\frac32}\,\|f\|_{\frac12,\Gamma}$$

if (3.61) holds.

Remark 3.20. If we extract the potential $U(x)$ from $\widetilde{\sigma}^L(x)$ according to (2.25), in many exterior points $x\in\Omega^c$, this approximation may efficiently be computed by clustering $e(x-y)$. The error in

$$\widetilde{U}^L(x) = \int_\Gamma e_m(x-y)\,\widetilde{\sigma}^L(y)\,ds_y$$

may be estimated by

$$\begin{aligned}|U(x)-\widetilde{U}^L(x)| &\le |U(x)-U^L(x)|+|U^L(x)-\widetilde{U}^L(x)|\\ &\le |U(x)-U^L(x)|+\Big|\int_\Gamma e(x,y)(\sigma^L-\widetilde{\sigma}^L)ds_y\Big| \qquad (3.67)\\ &\quad +\Big|\int_\Gamma |e(x,y)-e_m(x,y)|\,\widetilde{\sigma}^L\,ds\Big|.\end{aligned}$$

Combining (2.27), (3.47) we see that (3.61) ensures once more the optimal error bound (2.27) also for $U-\widetilde{U}^L$.

4 Iterative Solution and Complexity

4.1 General remarks

In Section 3 we saw that the cluster approximation of the kernel will not decrease the asymptotic rate of convergence of $\widetilde{\sigma}^L$ provided the order m of the cluster expansion increases logarithmically with h_L. We assumed there that the linear systems $\widetilde{\boldsymbol{A}}^L \underline{\widetilde{\sigma}}^L = \underline{f}$ are solved exactly. In practice, however, clustering methods are used with iterative methods like CG or GMRES with incomplete iterations. Since each iteration requires one matrix-vector multiplication $\underline{x} \longmapsto \widetilde{\boldsymbol{A}}^L \underline{x}$, which can be performed in $O(m^d N_L) = O(N_L(\log N_L)^d)$ operations, the solution must require no more than $O((\log N_L)^b)$ CG or GMRES iterations with some $b > 0$ to reduce the error to the order of the discretization error. It is not hard to see with (3.64) that $\widetilde{\boldsymbol{A}}^L$ is symmetric and that

$$\kappa = \mathrm{cond}_2(\widetilde{\boldsymbol{A}}^L) = O(h_L^{-1}) \text{ as } L \to \infty\,. \tag{4.1}$$

The CG method gives vectors $\underline{\sigma}_j^L$, $j = 0, 1, 2, \ldots$ with

$$\|\underline{\widetilde{\sigma}}^L - \underline{\sigma}_j^L\|_{\widetilde{\boldsymbol{A}}^L} \le 2\Big(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\Big)^j \|\underline{\widetilde{\sigma}}^L\|_{\widetilde{\boldsymbol{A}}^L}\,. \tag{4.2}$$

By (3.58), (3.59), the norm $\|\underline{\sigma}\|_{\widetilde{\boldsymbol{A}}^L} = (\widetilde{\boldsymbol{A}}^L \underline{\sigma}, \underline{\sigma})^{1/2}$ is equivalent to $\|\sigma\|_{-\frac{1}{2},\Gamma}$ where $(\cdot,\cdot)$ denotes the standard scalar product on $\mathbb{C}^{N_L}$.
Let $\sigma_j^L \in V^L$ denote the piecewise constant function associated with the vector $\underline{\sigma}_j^L$. Then (4.2) implies that the error of the j-th CG iterate σ_j^L satisfies

$$\begin{aligned}
\|\widetilde{\sigma}^L - \sigma_j^L\|_{-\frac{1}{2},\Gamma} &\le C\, \|\widetilde{\sigma}^L - \sigma_j^L\|_{0,\Gamma} = C\|\underline{\widetilde{\sigma}}^L - \underline{\sigma}_j^L\|_{\ell_2} \\
&\le\ C\big(1 - h_L^{\frac{1}{2}}\big)^j\, \|\underline{\widetilde{\sigma}}^L\|_{\ell_2} \\
&\le C\,\big(1 - h_L^{\frac{1}{2}}\big)^j\, h_L^{-\frac{1}{2}}\, \|\widetilde{\sigma}^L\|_{-\frac{1}{2},\Gamma} \\
&\le C\,\|f\|_{\frac{1}{2},\Gamma}\, h_L^{-\frac{1}{2}} \big(1 - h_L^{\frac{1}{2}}\big)^j\,.
\end{aligned} \tag{4.3}$$

We stop the CG procedure, once the error (4.3) is $O(h_L^{\frac{3}{2}})$, i.e. once $(1 - h_L^{\frac{1}{2}})^j < h_L^2$. Since $j \log(1 - \sqrt{h_L}) < -j\sqrt{h_L}$, this is satisfied in $j > 2|\log h_L| h_L^{-\frac{1}{2}} = O(N^{\frac{1}{4}} \log N)$ iterations, i.e. in a total of $O(N^{\frac{5}{4}}(\log N)^{d+1})$ operations. The situation is worse if GMRES is used for the solution, due to the weaker available convergence estimates.

To obtain an algorithm with log-linear complexity, we must precondition $\widetilde{\boldsymbol{A}}^L$. We describe here a preconditioner for $\widetilde{\boldsymbol{A}}^L$ which is based on Haar-multiwavelet bases of the subspaces V^L. In these bases, due to a result of Oswald [21], a condition number $\kappa = \mathrm{cond}_2(\widetilde{\boldsymbol{A}}^L) = O(L) = O(|\log h_L|)$ is achievable. We emphasize that the Haar basis is not used for matrix compression, but merely for preconditioning: the Haar basis does not have enough vanishing moments for optimal wavelet-compression [30]. However, its support is the smallest possible. We present the wavelets and the complexity estimate for both CG and GMRES with wavelet preconditioning in

Section 4.1. The main result states that Čebyšev-clustering with Haar wavelet preconditioning does give a $O(N(\log N)^b)$ complexity algorithm for weakly singular first kind BIEs on polyhedra.

The construction of Haar-wavelets used in [21] requires a sequence of nested triangulations $\mathcal{M}^0, \mathcal{M}^1, \ldots$ on Γ. Often, however, $\mathcal{M}^0$ is the finest mesh manageable in the computer and no refinements are possible. We show in Section 4.2 how to construct Haar-wavelet preconditioners on $\mathcal{M}^L$. In Section 4.3 we show how to construct Haar-wavelets on unstructured surface meshes $\mathcal{M}^0$ without any refinement at all based on a $O(N)$ agglomeration algorithm from [29].

4.2 Wavelet Preconditioning in $H^{-\frac{1}{2}}(\Gamma)$

On the polyhedron Γ with N_0 plane faces $\pi_j^0 \in \mathcal{M}^0$, which we assume for convenience to be triangles, we introduce a dyadic sequence $\{\mathcal{M}^\ell\}_{\ell=0}^\infty$ of meshes by regular refinement: each $\pi_j^\ell \in \mathcal{M}^\ell$ is obtained by subdividing a $\pi_j^{\ell-1} \in \mathcal{M}^{\ell-1}$ into 4 congruent triangles by connecting the mid-sides. By V^L we denote the piecewise constant functions on $\mathcal{M}^L$. We define for $\ell = 1, 2, \ldots$ the spaces W^ℓ via

$$W^\ell = \{\varphi \in V^\ell : \langle \varphi, \psi \rangle = 0 \quad \forall \psi \in V^{\ell-1}\} \tag{4.4}$$

and set $W^0 = V^0$. By P^ℓ: $L^2(\Gamma) \to V^\ell$ we denote the $L^2(\Gamma)$-projection:

$$\langle u - P^\ell u, v \rangle = 0 \quad \forall v \in V^\ell . \tag{4.5}$$

Given a function $u^L \in V^L$, we have the multilevel decomposition

$$u^L = \sum_{\ell=0}^{L} w^\ell, \quad w^\ell = (P^\ell - P^{\ell-1})\, u^L \tag{4.6}$$

and the norm equivalence

$$\|u^L\|^2_{L^2(\Gamma)} = \sum_{\ell=0}^{L} \|w^\ell\|^2_{L^2(\Gamma)}, \quad u^L \in V^L . \tag{4.7}$$

(4.6) and (4.7) also hold for $L = \infty$, where V^L is replaced by $L^2(\Gamma)$:

$$\forall u \in L^2(\Gamma): \quad \|u\|^2_{L^2(\Gamma)} = \sum_{\ell=0}^{\infty} \|w^\ell\|^2_{L^2(\Gamma)} = \sum_{\ell=0}^{\infty} \|(P^\ell - P^{\ell-1})\, u\|^2_{L^2(\Gamma)} \tag{4.8}$$

where $P^{-1} := 0$. We may therefore write

$$V^L = \bigoplus_{\ell=0}^{L} W^\ell, \quad L^2(\Gamma) = \bigoplus_{\ell=0}^{\infty} W^\ell \tag{4.9}$$

the decomposition being orthogonal in $L^2(\Gamma, ds)$. The increments $W^\ell = V^\ell \cap (V^{\ell-1})^\perp$ are spanned by wavelets ψ_j^ℓ which are translates and dilates of the mother-wavelets ψ_j^1 shown in Fig. 4.1

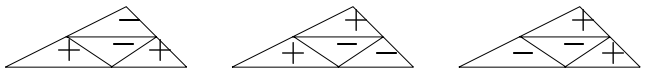

Figure 4.1: Triangular polyhedral side $\pi_j^0 \in \mathcal{M}^0$, subdivision into 4 congruent triangles $\pi_j^1 \in \mathcal{M}^1$ and 3 mother-wavelets ψ_j^1 on π_j^1

Evidently, the multiwavelets ψ_j^ℓ are orthonormal in $L^2(\Gamma, ds)$. Any function $u \in L^2(\Gamma, ds)$ can be expanded in the wavelet basis:

$$u = \sum_{\ell=0}^{\infty} \sum_{j \in J^\ell} u_j^\ell \, \psi_j^\ell, \quad u_j^\ell = \langle u, \psi_j^\ell \rangle \tag{4.10}$$

and we have obviously also

$$w^\ell = R_\ell \, u = (P_\ell - P_{\ell-1}) \, u = \sum_{j \in J^\ell} u_j^\ell \, \psi_j^\ell \, . \tag{4.11}$$

A basic tool in the theory of multilevel schemes are the norm equivalences akin to (4.8) in the scale $H^s(\Gamma)$, $s \neq 0$, of Sobolev spaces. The central result of relevance for preconditioning in $H^{-\frac{1}{2}}(\Gamma)$ is due to Oswald [21]:

Proposition 4.1. *There are $c_1, c_2 > 0$ depending only on the shape of Γ such that for any $|s| < \frac{1}{2}$*

$$\forall u \in H^s(\Gamma) : \; c_1 \|u\|^2_{H^s(\Gamma)} \leq \sum_{\ell=0}^{\infty} 2^{2\ell s} \|R_\ell \, u\|^2_{L^2(\Gamma)} \leq c_2 \|u\|^2_{H^s(\Gamma)} \, . \tag{4.12}$$

In the limiting case $s = -\frac{1}{2}$ holds

$$\forall u^L \in V^L : \; c_1 \|u^L\|^2_{H^{-\frac{1}{2}}(\Gamma)} \leq \sum_{\ell=0}^{L} 2^{-\ell} \|R_\ell \, u^L\|^2_{L^2(\Gamma)} \leq c_2 (L+1)^2 \, \|u^L\|^2_{H^{-\frac{1}{2}}(\Gamma)} \tag{4.13}$$

where c_1, c_2 are independent of L.

Oswald also shows in [21] that the factor $(L+1)^2$ cannot be removed in general.

For preconditioning, we proceed as follows: let $\boldsymbol{A}^\Phi$, $\widetilde{\boldsymbol{A}}^\Phi$ denote the stiffness matrix without and with multipole compression in the standard basis $\Phi = \{\varphi_j^L\}$, $V^L = \mathrm{span}\{\varphi_j^L\}$, and let $\boldsymbol{A}^\Psi$, $\widetilde{\boldsymbol{A}}^\Psi$ denote these matrices transformed to the wavelet basis $\Psi = \{\psi_j^\ell : 0 \leq \ell \leq L, j \in J^\ell\}$. The basis transformation can be done in $O(N_L)$ operations and is denoted symbolically by $\boldsymbol{W}$: we have

$$\boldsymbol{W} \underline{x}^\Phi = \underline{x}^\Psi, \;\; \underline{x}^\Phi = \boldsymbol{W}^{-1} \, \underline{x}^\Psi = \boldsymbol{W}^\top \, \underline{x}^\Psi \tag{4.14}$$

for $\underline{x}^\Phi$, $\underline{x}^\Psi \in \mathbb{R}^{N_L}$ and $\boldsymbol{W}^{-1} = \boldsymbol{W}^\top$ since Ψ is $L^2(\Gamma)$-orthonormal.

To solve $\underline{\boldsymbol{A}}^\Phi \, \underline{\sigma}^\Phi = \underline{\widetilde{f}}^\Phi$, we transform it to the Wavelet basis Ψ:

$$\begin{array}{ccccc} \underbrace{\boldsymbol{W} \, \widetilde{\boldsymbol{A}}^\Phi \, \boldsymbol{W}^\top} & \underbrace{\boldsymbol{W} \, \underline{x}^\Phi} & = & \underbrace{\boldsymbol{W} \, \underline{\widetilde{b}}^\Phi} & \\ \widetilde{\boldsymbol{A}}^\Psi & \underline{\sigma}^\Psi & = & \underline{\widetilde{f}}^\Psi \, . & \end{array} \tag{4.15}$$

Now Proposition 4.1 implies immediately

Proposition 4.2. *Assume* (3.57) *and denote by* $\boldsymbol{C}$ *the diagonal matrix*

$$\boldsymbol{C} = \mathrm{diag}\{2^{-\frac{\ell}{2}}\,\delta_{ij} : i,j \in J^\ell,\ 0 \le \ell \le L\}\,.$$

Then we have for the matrix $\widehat{\boldsymbol{A}} = \boldsymbol{C}^{-1}\,\widetilde{\boldsymbol{A}}^{\,\Psi}\,\boldsymbol{C}^{-1}$ *and for all* $\underline{y},\underline{x} \in \mathbb{C}^{N_L}$

$$Re\,\underline{x}^H\,\widehat{\boldsymbol{A}}\,\underline{x} \ge C_1(L+1)^{-2}\,\|\underline{x}\|_{\ell_2}^2\,, \tag{4.16}$$

$$|\underline{x}^H\,\widehat{\boldsymbol{A}}\,\underline{y}| \le C_2\|\underline{x}\|_{\ell_2}\,\|\underline{y}\|_{\ell_2}\,. \tag{4.17}$$

Proof. We have for every $\underline{u},\underline{v} \in \mathbb{C}^{N_L}$ with (4.13)

$$|\widetilde{a}(u^L,v^L)| \le C\,\|u^L\|_{H^{-\frac{1}{2}}(\Gamma)}\|v^L\|_{H^{-\frac{1}{2}}(\Gamma)} \le \frac{c}{c_1}\,\|\boldsymbol{C}\,\underline{u}\|_{\ell_2}\,\|\boldsymbol{C}\,\underline{v}\|_{\ell_2}$$

and

$$Re\,\widetilde{a}(u^L,u^L) \ge C\,\|u^L\|^2_{H^{-\frac{1}{2}}(\Gamma)} \ge \frac{C}{c_2(L+1)^2}\,\|\boldsymbol{C}\,\underline{u}\|^2_{\ell_2}\,.$$

It follows that there are constants C_1, C_2 independent of L such that for every $\underline{u},\ \underline{v} \in \mathbb{C}^{N_L}$

$$|\underline{u}^H\,\widetilde{\boldsymbol{A}}^{\,\Psi}\,\underline{v}| \le C_2\|\boldsymbol{C}\underline{u}\|_{\ell_2}\,\|\boldsymbol{C}\,\underline{v}\|_{\ell_2} \quad \text{and} \quad Re\,\underline{u}^H\,\widetilde{\boldsymbol{A}}^{\,\Psi}\,\underline{u} \ge \frac{C_1}{(L+1)^2}\,\|\boldsymbol{C}\,\underline{u}\|^2_{\ell_2}\,.$$

Setting $\underline{x} = \boldsymbol{C}\,\underline{u}$, $\underline{y} = \boldsymbol{C}\,\underline{v}$, (4.16) and (4.17) follow. □

We conclude that if $\widetilde{\boldsymbol{A}}$ is hermitian,

$$\mathrm{cond}_2(\widehat{\boldsymbol{A}}) = \lambda_{\max}(\widehat{\boldsymbol{A}})/\lambda_{\min}(\widehat{\boldsymbol{A}}) \sim \frac{C_2}{C_1}\,(L+1)^2\,. \tag{4.18}$$

Theorem 4.3. *If the linear system* (4.15) *is solved iteratively by either CG (if* $\widetilde{\boldsymbol{A}}$ *is symmetric) or by GMRES with restart after 1 iteration, applied to the preconditioned matrix* $\widehat{\boldsymbol{A}}$*, generating the sequence* $\{\underline{\sigma}_{(j)}\}_{j=0}^{\infty}$ *with starting vector* $\underline{u}_{(0)} = \underline{0}$*, and by* $\{\sigma^L_{(j)}\}_{j=0}^{\infty}$ *the sequence of approximate solutions. Then there holds the error bound*

$$\|\sigma^L - \sigma^L_{(j)}\|_{H^{-\frac{1}{2}}(\Gamma)} \le Ch_L^{\frac{3}{2}} \tag{4.19}$$

provided the number j *of iterations satisfies*

$$j \ge c_* L^a,\ \ a = \begin{cases} 2 \text{ for CG} \\ 5 \text{ for GMRES} \end{cases} \tag{4.20}$$

for some $c_* > 0$ *large enough.*

Proof. We have for CG with (4.18) in the wavelet basis Ψ:

$$\|\underline{\sigma}^L - \underline{\sigma}^L_{(j)}\|_{\widetilde{\boldsymbol{A}}^L} \le 2\Big(\frac{\sqrt{\mathrm{cond}_2(\widehat{\boldsymbol{A}})}-1}{\sqrt{\mathrm{cond}_2(\widehat{\boldsymbol{A}})}+1}\Big)^j \|\underline{\sigma}^L - \underline{\sigma}^L_{(0)}\|_{\widetilde{\boldsymbol{A}}^L} \le C\Big(1-\frac{C}{L+1}\Big)^j \|\underline{\sigma}^L\|_{\widetilde{\boldsymbol{A}}^L} \overset{!}{\le} C\, h_L^{\frac{3}{2}}.$$

Since $h_L = O(2^{-L})$, the claim follows for CG with (4.13).

For GMRES, we use (4.16), (4.17) which imply

$$\lambda_{\min}\big((\widehat{\boldsymbol{A}} + \widehat{\boldsymbol{A}}^H)/2\big) \ge C_1(L+1)^{-2},$$

and [11] who proved

$$\|\underline{\sigma}^L - \underline{\sigma}^L_{(j)}\|_{\ell_2} \le \Big(1 - \frac{C_1^2}{C_2^2(L+1)^4}\Big)^{j/2} \|\underline{\sigma}^L\|_{\ell_2}.$$

It follows that $\|\sigma^L - \sigma^L_{(j)}\|_{H^{-\frac{1}{2}}(\Gamma)} \le C\, h_L^a$ if $j \ge c_*(L+1)^5$ with $c_* > 0$ sufficiently large (depending on a). □

Remark 4.4. The exponent $a = 5$ for GMRES in (4.20) is likely not optimal.

We can now estimate the complexity of the algorithm. Note that in practice, the matrix $\widehat{\boldsymbol{A}}$ is never formed - we apply instead PCCG with preconditioner $\boldsymbol{C}^{-1}\boldsymbol{W}$ directly to $\widetilde{\boldsymbol{A}}^{\Phi}$ which is realized by a clustering scheme.

Proposition 4.5. *The total work for the iterative solution of the linear system*

$$\widetilde{\boldsymbol{A}}\,\widetilde{\underline{\sigma}}^L = \widetilde{\underline{b}}$$

(to the accuracy of the discretization error of full Galerkin) by CG or GMRES with multilevel preconditioner $\boldsymbol{C}^{-1}\boldsymbol{W}$ is bounded by

$$C\, N_L(\log N_L)^{a+b} \tag{4.21}$$

operations with

$$a = \begin{cases} 2 \text{ for CG} \\ 5 \text{ for GMRES} \end{cases}, \quad b = \begin{cases} 2 \text{ for spherical harmonics,} \\ 3 \text{ for Čebyšev clustering.} \end{cases}$$

If the iteration is run to a fixed tolerance τ rather than to $O(h^a)$, $a+b$ in (4.21) is reduced by one.

Remark 4.6. We assumed here that the nearfield part of matrix $\widetilde{\boldsymbol{A}}$ can be computed exactly in $O(N_L)$ operations. If this is not possible, the quadrature scheme in [22] gives consistent approximations in $O(N_L(\log N_L)^4)$ operations.

4.3 Coarsening by Agglomeration

The multiwavelet basis $\{\psi_j^\ell\}_{\ell=0}^L$ of V^L used in the preconditioner $\boldsymbol{C}$ in Proposition 4.2 is only effective if $L > 1$. Often, however, already the mesh $\mathcal{M}^0$ describing the geometry has $N_0 = O(10^5)$ panels π_i^0. In such cases, the preconditioner $\boldsymbol{C}$ cannot improve the condition number. To deal with this case, we extend the decomposition $V^L = W^0 \oplus \cdots \oplus W^L$ to levels $\ell < 0$. This coarsening is conveniently achieved by using the hierarchy of clusters in the cluster tree $\mathcal{T}(\mathcal{M}^0)$ constructed for the farfield acceleration. In what follows, we denote by

$$\mathcal{T} = \mathcal{T}(\mathcal{M}^0) \tag{4.22}$$

an η-admissible cluster tree on $\mathcal{M}^0$. Some definitions follow:

Definition 4.7.

1. *The depth $d_\mathcal{T}$ of the cluster tree $\mathcal{T}$ is defined by*

$$d_\mathcal{T} = \max_{\tau\in\mathcal{T}} \left\{\ell \in \mathbb{N}_0 : \tau \subsetneq \tau_{i_1} \subsetneq \tau_{i_2} \subsetneq \cdots \subsetneq \tau_{i_\ell} = \mathcal{M}^0,\ \tau_{i_1}, \tau_{i_2}, \ldots \tau_{i_\ell} \in \mathcal{T}(\mathcal{M}^0)\right\}. \tag{4.23}$$

2. *The level ℓ_τ of a cluster $\tau \in \mathcal{T}(\mathcal{M}^0)$ is defined by*

$$\ell_\tau = -d_\mathcal{T} + \max_{\ell\in\mathbb{N}_0} \left\{\tau \subsetneq \tau_{i_1} \subsetneq \tau_{i_2} \cdots \subsetneq \tau_{i_\ell} = \mathcal{M}^0,\ \tau_{i_1}, \tau_{i_2} \ldots,\ \tau_{i_\ell} \in \mathcal{T}(\mathcal{M}^0)\right\}. \tag{4.24}$$

3. *The agglomerated panel π_j^ℓ associated with a cluster $\tau_j^\ell \in \mathcal{T}(\mathcal{M}^0)$ of level $\ell < 0$ is defined by*

$$\pi_j^\ell = \bigcup \left\{\overline{\pi^0} \in \mathcal{M}^0 : \pi^0 \in \tau_j^\ell\right\}. \tag{4.25}$$

   We denote a cluster $\tau \in \mathcal{T}(\mathcal{M}^0)$ of level ℓ also by τ^ℓ.

4. *For $\ell < 0$ the coarsened mesh $\mathcal{M}^\ell$ is the union of all agglomerated panels π_j^ℓ:*

$$\mathcal{M}^\ell = \{\pi_j^\ell : j \in J^\ell\},\ -d_\mathcal{T} \le \ell < 0\,. \tag{4.26}$$

Evidently, the root of $\mathcal{T}(\mathcal{M}^0)$ satisfies

$$\{\Gamma\} = \mathrm{root}\big(\mathcal{T}(\mathcal{M}^0)\big) = \mathcal{M}^{-d_\mathcal{T}}\,. \tag{4.27}$$

4.3.1 Agglomeration Procedure

The agglomerated wavelet basis $\{\psi_{\tau,j}\}$ is constructed from the scaling functions $\{\varphi_i^L\}_{i=1}^{N_0}$ by the following agglomeration procedure. In a first step, we compute for each cluster $\tau \in \mathcal{T}$ with $\mathrm{child}(\tau) = \emptyset$ the piecewise constant orthonormal basis functions φ_τ ($(\varphi_\tau, \varphi_{\tau'}) = \delta_{\tau\tau'}$)

$$\varphi_\tau(\underline{x}) = \begin{cases} 1/\sqrt{|\tau|}, & \underline{x} \in \tau \\ 0, & \text{else} \end{cases} \tag{4.28}$$

with $|\tau| = \int_\tau ds_{\underline{x}}$. Afterwards for each cluster τ with $\mathrm{child}(\tau) \neq \emptyset$ the wavelets $\psi_\tau = \{\psi_{\tau,j}\}_{j=1}^{|\mathrm{child}(\tau)|-1}$ and the coarsened scaling function φ_τ are computed by the local wavelet transformation $\boldsymbol{M}_\tau$. The constant normed function φ_τ with $\mathrm{supp}(\varphi_\tau) = \tau$ is needed to get the

wavelets on the next lower level. At the end of this agglomeration the recursion wavelet basis consists of the functions

$$\varphi_{\mathrm{root}(\mathcal{T})} \quad \text{and} \quad \{\psi_{\tau,j}\}_{(\tau,j)\in\mathcal{J}} \tag{4.29}$$

where $\mathcal{J} = \{(\tau, j) : \tau \in \mathcal{T} \wedge \mathrm{child}(\tau) \neq \emptyset,\ 1 \leq j < |\mathrm{child}(\tau)|\}$. The construction of the agglomerated wavelet basis is realized by Algorithm 4.1.

Algorithm 4.1

for $l = 0$ down to $L_{\mathcal{T}}$
  for all $\tau \in \mathcal{T}$ with $l_\tau = l$
    if $\mathrm{child}(\tau) = \emptyset$
      compute φ_τ;
    else

$$\text{compute } \begin{pmatrix} \varphi_\tau \\ \psi_\tau \end{pmatrix} = \boldsymbol{M}_\tau^\top \begin{pmatrix} \varphi_{\tau_{i_1}} \\ \vdots \\ \varphi_{\tau_{i_{|\mathrm{child}(\tau)|}}} \end{pmatrix}, \tau_{i_\lambda} \in \mathrm{child}(\tau)$$

4.3.2 Local transformation $\boldsymbol{M}_\tau$

For each tree $\mathcal{T}(\mathcal{M}^0)$ with $|\mathrm{child}(\mathcal{T})| > 1$ we can construct the agglomerated wavelet basis of the space V^0 of piecewise constants by applying Algorithm 4.1 and the local transformations $\boldsymbol{M}_\tau$.

The local transformation $\boldsymbol{M}_\tau$ converts the scaling functions $\varphi_{\tau_{i_\lambda}}$ with $\tau_{i_\lambda} \in \mathrm{child}(\tau)$ into the local wavelet basis $\psi_\tau = \{\psi_{\tau,j}\}_{j=1}^{|\mathrm{child}(\tau)|-1}$ and the coarsened scaling function φ_τ:

$$\begin{pmatrix} \varphi_\tau \\ \psi_\tau \end{pmatrix} = \boldsymbol{M}_\tau^\top \begin{pmatrix} \varphi_{\tau_{i_1}} \\ \vdots \\ \varphi_{\tau_{i_{|\mathrm{child}(\tau)|}}} \end{pmatrix}. \tag{4.30}$$

To get an orthonormal wavelet basis of V^0 the local transformation matrix $\boldsymbol{M}_\tau = (\underline{m}_1^\tau, \ldots, \underline{m}_{|\mathrm{child}(\tau)|}^\tau)$ has to satisfy

$$\boldsymbol{M}_\tau^\top \boldsymbol{M}_\tau = I\,. \tag{4.31}$$

For each cluster τ in the tree $\mathcal{T}$ we compute the local transformation matrix $\boldsymbol{M}_\tau$ by defining $\widetilde{\boldsymbol{M}}_\tau = (\underline{m}_1^\tau,\ \widetilde{\underline{m}}_2^\tau, \ldots, \widetilde{\underline{m}}_{|\mathrm{child}(\tau)|}^\tau)$ with

$$(\underline{m}_1^\tau)^\top = \frac{1}{\sqrt{|\tau|}}(\sqrt{|\tau_{i_1}|}, \ldots, \sqrt{|\tau_{i_{|\mathrm{child}(\tau)|}}|}), \quad \tau_{i_\lambda} \in \mathrm{child}(\tau)$$

and $\widetilde{\underline{m}}_2^\tau, \ldots, \widetilde{\underline{m}}_{|\mathrm{child}(\tau)|}^\tau$ such that

$$\det(\widetilde{\boldsymbol{M}}_\tau) \neq 0, \quad (\underline{m}_1^\tau)^\top \widetilde{\underline{m}}_i^\tau = 0, \quad 2 \leq i \leq |\mathrm{child}(\tau)|.$$

Applying the singular value decomposition (SVD) to the vectors $\underline{\widetilde{m}}_2^\tau,\ldots,\underline{\widetilde{m}}_{|\mathrm{child}(\tau)|}^\tau$, we get the matrix $\boldsymbol{M}_\tau$

$$(\boldsymbol{U}_\tau,\boldsymbol{S}_\tau,\boldsymbol{V}_\tau)=\mathrm{SVD}((\underline{\widetilde{m}}_2^\tau,\ldots,\underline{\widetilde{m}}_{|\mathrm{child}(\tau)|}^\tau)),\quad \boldsymbol{M}_\tau=(\underline{m}_1^\tau,\,\boldsymbol{U}_\tau) \tag{4.32}$$

which satisfies (4.31).

Proposition 4.8. *With the local transformation matrix $\boldsymbol{M}_\tau$ defined above, we get a local basis φ_τ, ψ_τ which is orthonormal with respect to the surface measure on Γ, i.e.*

$$\|\varphi_\tau\|_{L^2(\Gamma)} = 1 \tag{4.33}$$
$$(\varphi_\tau,\psi_{\tau,j}) = 0 \qquad 1\le j<|\mathrm{child}(\tau)| \tag{4.34}$$
$$(\psi_{\tau,j},\psi_{\tau,j'}) = \delta_{jj'} \qquad 1\le j,j'<|\mathrm{child}(\tau)|. \tag{4.35}$$

In our implementation, we use the matrix $\widetilde{\boldsymbol{M}}_\tau$ in Assertion 4.9.

Assertion 4.9. *The matrix*

$$\widetilde{\boldsymbol{M}}_\tau = \begin{bmatrix} \widetilde{m}_1^\tau & -\widetilde{m}_2^\tau & 0 & 0 & \cdots & 0\\ \widetilde{m}_2^\tau & \widetilde{m}_1^\tau & -\widetilde{m}_3^\tau & 0 & \ldots & 0\\ \widetilde{m}_3^\tau & 0 & \widetilde{m}_2^\tau & -\widetilde{m}_4^\tau & & \vdots\\ \vdots & \vdots & & \ddots & \ddots & 0\\ \widetilde{m}_{n-1}^\tau & 0 & & & \widetilde{m}_{n-2}^\tau & -\widetilde{m}_n^\tau\\ \widetilde{m}_n^\tau & 0 & & \cdots & 0 & \widetilde{m}_{n-1}^\tau \end{bmatrix} \tag{4.36}$$

with $\tau\in\mathcal{T}$, $\tau_{i_\lambda}\in\mathrm{child}(\tau)$, $\widetilde{m}_\lambda^\tau=\sqrt{|\tau_{i_\lambda}|/|\tau|}$ and $n=|\mathrm{child}(\tau)|$ has full rank.

Remark 4.10. The local transformation (4.30) can be seen as an application of the lifting scheme presented in [31, 32] or the stable completion in [3, 4, 7]. We start with the scaling function ϕ_τ and the wavelets

$$\widetilde{\psi}_{\tau,j}=(\underline{\widetilde{m}}_{j+1}^\tau)^\top\begin{pmatrix}\varphi_{\tau_{i_1}}\\ \vdots\\ \varphi_{\tau_{i_{|\mathrm{child}(\tau)|}}}\end{pmatrix}\quad 1\le j<|\mathrm{child}(\tau)|$$

defined by the matrix $\widetilde{\boldsymbol{M}}_\tau$ and $\{\varphi_{\tau_\lambda}\}$. These wavelets are lifted to an orthonormal basis on Γ with vanishing mean value with respect to the surface measure ds on Γ. This is done using the singular value decomposition (4.32).

Remark 4.11. In case of a binary tree, the local transformation matrix $\boldsymbol{M}_\tau$ is

$$\boldsymbol{M}_\tau=\begin{bmatrix}\sqrt{|\tau_1|/|\tau|} & -\sqrt{|\tau_2|/|\tau|}\\ \sqrt{|\tau_2|/|\tau|} & \sqrt{|\tau_1|/|\tau|}\end{bmatrix}$$

for $\tau_1,\tau_2\in\mathrm{child}(\tau)$. Then the singular value decomposition can be omitted.

4.3.3 Properties of the agglomerated wavelet basis

For any triangulation $\mathcal{M}^0$ on Γ, Algorithm 4.1 generates an agglomerated wavelet basis. The forward and backward transformation of the pyramid scheme for vectors $\underline{f}^{\varphi}$ and $\underline{f}^{\psi}$ are standard and omitted, since they are almost identical to Algorithm 4.1. The agglomerated wavelet basis has desirable properties:

Proposition 4.12. *The wavelet basis obtained from Algorithm* 4.1 *is an* $L^2(\Gamma, ds)$ *orthonormal basis of* V_N.

a) *The agglomerated wavelets fulfill the vanishing moment property*

$$\int_\Gamma \psi_{\tau,j}(\underline{x}) ds_{\underline{x}} \;=\; 0 \qquad \text{for } (\tau, j) \in \mathcal{J} \tag{4.37}$$

with $\mathcal{J}$ *defined as in* (4.29).

b) *The agglomerated wavelet basis satisfies Parseval's equation in* $L^2(\Gamma, ds)$.

$$\|u\|^2_{L^2(\Gamma)} \;=\; (u, \varphi_{\mathrm{root}(\mathcal{T})})^2 + \sum_{(\tau,j)\in\mathcal{J}} (u, \psi_{\tau,j})^2 \tag{4.38}$$

for all $u \in V_N$.

c) *With* $W_l = \mathrm{span}\{\psi_{\tau,j} : l_\tau = l-1, 1 \le j < |\mathrm{child}(\tau)|\}$, $l > -d_{\mathcal{T}}$, *it holds*

$$V_N \;=\; W_{-d_{\mathcal{T}}} \oplus W_{-d_{\mathcal{T}}+1} \oplus \ldots \oplus W_0 \tag{4.39}$$

where we have set $W_{-d_{\mathcal{T}}} = \mathrm{span}\{\varphi_{\mathrm{root}(\mathcal{T})}\}$

Equation (4.38) is a consequence of the clusters on the same level being disjoint and of the orthogonality of the wavelets between different levels. The orthogonality between different levels follows from (4.34).

Remark 4.13. If we refine $\mathcal{M}^0$ beyond level $l = 0$ by regular subdivision of each $\pi_i \in \mathcal{M}^0$, the corresponding spaces of piecewise constants are dense in $L^2(\Gamma, ds)$ and the finite sum in Parseval's equality (4.38) can be extended to an infinite one as for example in [19, 24].

Remark 4.14. It is an interesting open problem to establish an analog of Proposition 4.1 for the agglomerated wavelet basis. Below, we investigate the diagonal preconditioning in the agglomerated wavelet basis numerically.

4.3.4 Complexity of the transformation

In this section the complexity of Algorithm 4.1 is estimated. In a first step of the algorithm we generate the cluster tree $\mathcal{T}$. With mild assumptions on the geometry of Γ, we see that we can compute a cluster tree $\mathcal{T}$ with $d_{\mathcal{T}} = O(\log N_0)$ (see [14]). To insert the leafs π_i into the cluster tree we need for each leaf at most $d_{\mathcal{T}} = O(\log N_0)$ operations. Therefore, we can compute the cluster tree $\mathcal{T}$ for N_0 leafs in $O(N_0 \log N_0)$ operations. The constant depends on a mild regularity condition on the surface (see [17, 29] for details) which is satisfied for the domains in Figure 4.2 uniformly in the number of slits. With this cluster tree we apply Algorithm 4.1. Then we have (see [29])

Proposition 4.15. *Algorithm* 4.1 *takes* $W_{tot} = O(N_0)$ *operations.*

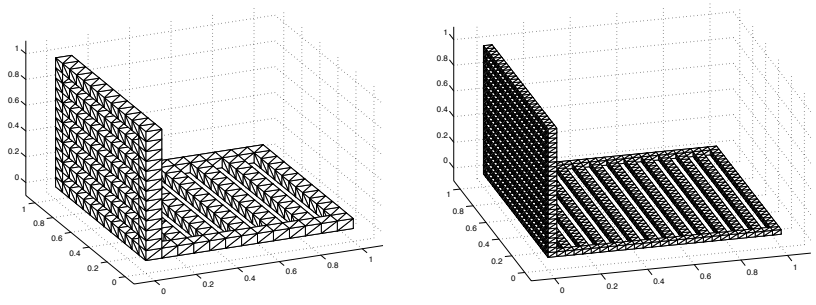

Figure 4.2: L-shaped domains with 6 and 13 slits on each side.

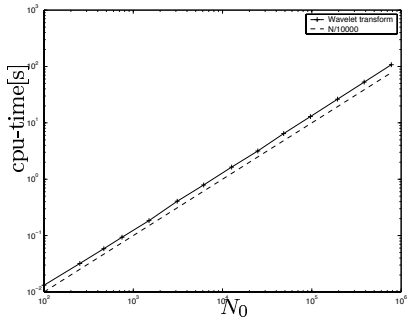

Figure 4.3: cpu-time to compute the cluster tree for the L-shaped domains and to apply the pyramid scheme to a vector versus the number of degrees of freedom.

We illustrate in 4.3 the result of Proposition 4.13. The wavelet transformation is applied to a vector in the one scale basis. The diagram shows the cpu-time for the pyramid scheme for the L-shaped domain with slits. The thickness of the L-shaped domain and the slits is always one triangle. Therefore an increase of the degrees of freedom in the L-shaped domain problem induces also more slits and changes consequently the geometry. This leads to a series of domains where in Fig. 4.2 the domains with 6 ($N = 1500$) and 13 slits ($N = 6148$) are plotted. We see that the cpu-time behaves like $O(N)$ as stated in Proposition 4.13.

5 Numerical Results

In this section we will discuss different numerical experiments for the agglomeration preconditioner proposed in Section 4. In addition to the normed one scale basis introduced in Section 2.3

$$\Phi^l := \{\varphi_j^l : \varphi_j^l = |\pi_j^l|^{-\frac{1}{2}} \chi_{\pi_j^l}, 1 \leq j \leq N_l\} \tag{5.1}$$

we define a new basis by

$$\tilde{\Phi}^l := \{\tilde{\varphi}_j^l := \chi_{\pi_j^l}, 1 \leq j \leq N_l\}. \tag{5.2}$$

For convenience we will omit the level l in our further explanations since in our experiments we choose $l = 0$ and construct the wavelets by agglomeration as explained in Section 4.3.

All experiments are based on the cluster approximation of the stiffness matrix in the basis $\tilde{\Phi}$

$$(\widetilde{\mathbf{A}})_{ji} \;=\; \int_\Gamma \int_\Gamma \tilde{\varphi}_j(x) k_m(x,y) \tilde{\varphi}_i(y)\, ds_y ds_x \,. \tag{5.3}$$

The different matrices in our tests are never formed explicit but a combination of the cluster approximation $\widetilde{\mathbf{A}}$ the transformation $\mathbf{D}$ which transforms a vector given in the basis $\tilde{\Phi}$ to a vector in the Φ basis

$$\mathbf{D}\underline{x}^{\tilde{\Phi}} = \underline{x}^{\Phi} \tag{5.4}$$

and the wavelet transformation $\mathbf{W}$ of Section 4.

The test problem is the interior Dirichlet problem

$$\begin{aligned} \Delta u &= 0 \qquad \text{in } \Omega \\ u &= f \qquad \text{on } \Gamma = \partial\Omega \end{aligned} \tag{5.5}$$

for $f = 1/\sqrt{(x_1 - 1.001)^2 + (x_2 - 1.001)^2 + (x_3 - 1.001)^2}$ and different domains $\Omega \subset \mathbb{R}^3$ where we measure the iteration numbers of GMRes [2]. Convergence is achieved if the relative residual is smaller than 10^{-10}. In our experiments we solved this problem on a Sun UltraSPARC-II 336 MHz with 1 GB memory and used the GNU compiler 2.95.2.1.

G_1 The first geometry is the unit cube with a uniform grid and the refinement levels from 0 up to 6. On level 0 each side consists of two triangles. The refinement is done by connecting the edge midpoints of each triangle which leads to four smaller triangles. With this we get the problem sizes $N_0 = 12$, 48, 192, 768, 3072, 12288 and 49152. Although the geometry is obtained by refining the cube on level 0 we construct all wavelets by agglomeration using a binary tree.

G_2 The second problem is the same as in Section 4.3.4 and consists of a series of different geometries. Each geometry is a L-shaped domain with a uniform grid and n slits of the size of a triangle on each side. In Figure 4.2 the geometries for $n = 6, 13$ are plotted. The problem (5.5) is solved for $n = 1$, 2, 3, 4, 6, 9, 13, 19, 27 and 38 with $N_0 = 100$, 252, 468, 748, 1500, 3108, 6148, 12628, 24852 and 48348.

The first preconditioner tested is the one proposed in Proposition 4.2. There we assume that the relation between the support sizes is 4. Since we are using a binary tree the relation of the support size of a cluster to the support size of its children is approximately 2. The advantage of a binary tree is the explicitly given local transformation matrix (see Remark 4.11). Adapting $\mathbf{C}$ to this situation we replace 2 by $\sqrt{2}$ and introduce a new parameter at our disposal. With this we get the preconditioner P_1

$$\mathbf{C}_t \;=\; \operatorname{diag}\{\sqrt{2}^{-(l_\tau + d_\mathcal{T})t} \delta_{ij} : i,j \in J^l, -d_\mathcal{T} \le l \le 0\}. \tag{5.6}$$

With the transformation $\mathbf{W}$ to the wavelet basis we have to solve

$$\mathbf{A}_t^{P_1}\underline{y} = \mathbf{C}_t\mathbf{W}\mathbf{D}^{-1}\widetilde{\mathbf{A}}\mathbf{D}^{-1}\mathbf{W}^\top\mathbf{C}_t\underline{y} = \mathbf{C}_t\mathbf{W}\mathbf{D}^{-1}\underline{b}$$

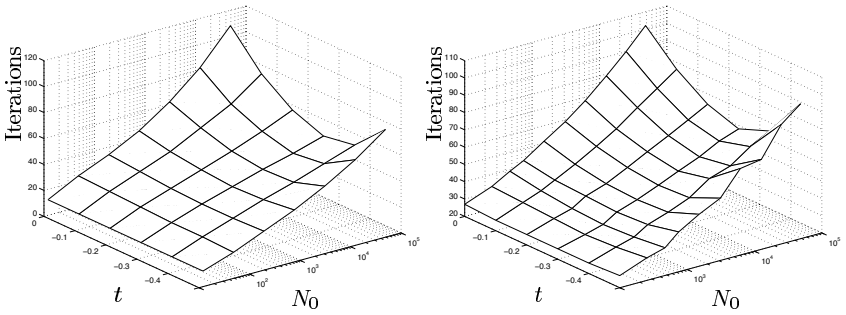

Figure 5.1: Number of GMRes iterations versus number of degrees of freedom and t for G_1 (left) and G_2 (right) with the preconditioner P_1. $t = 0$ corresponds to no preconditioning.

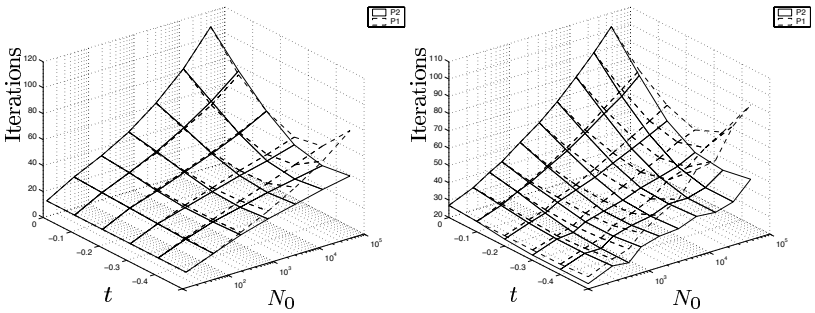

Figure 5.2: Number of GMRes iterations versus number of degrees of freedom and t for G_1 (left) and G_2 (right) with the preconditioners P_1 and P_2.

and then to compute $\underline{x} = \mathbf{D}^{-1}\mathbf{W}^\top \mathbf{C}_t \underline{y}$. The test problem (5.5) is solved for $-0.5 \leq t \leq 0$. With this preconditioner the iteration number of GMRes is reduced substantially as shown in Figure 5.1. Accordingly to the theory the minimal iteration number should be achieved for $t = -0.5$ (Proposition 4.2) and not for $t \approx -0.3$ as obtained in the experiment. The reason for this deviation lies in the agglomeration process. There it is not possible to ensure that the relation of the support size of a cluster to its children is exactly 2. We overcome this problem by replacing the approximated relative cluster size $\sqrt{2}^{-(l_\tau + d_\mathcal{T})}$ by the exact relative cluster size $\sqrt{|\tau_j^l|/|\Gamma|}$. With this we get the second preconditioner P_2

$$\tilde{\mathbf{C}}_t \;=\; \operatorname{diag}\left\{ \sqrt{\frac{|\tau_j^l|}{|\Gamma|}}^{t} \delta_{ij} : i,j \in J^l, -d_\mathcal{T} \leq l \leq 0 \right\} \tag{5.7}$$

where $\operatorname{supp}(\psi_j^l) = \tau_j^l$. Then the equation system looks like

$$\mathbf{A}_t^{P_2} \underline{y} = \tilde{\mathbf{C}}_t \mathbf{W} \mathbf{D}^{-1} \widetilde{\mathbf{A}} \mathbf{D}^{-1} \mathbf{W}^\top \tilde{\mathbf{C}}_t \underline{y} = \tilde{\mathbf{C}}_t \mathbf{W} \mathbf{D}^{-1} \underline{b}$$

with $\underline{x} = \mathbf{D}^{-1}\mathbf{W}^\top \tilde{\mathbf{C}}_t \underline{y}$. This generalization of the preconditioner P_1 leads to a reduction of the iteration number for G_1 and G_2. Further more the minimal iteration number is achieved for $t \approx -0.5$ which confirms the theory of Section 4.2. A comparison between the two preconditioners P_1 and P_2 for G_1 and G_2 can be seen in Figure 5.2. For $t = 0$ the iteration number is the same since $\mathbf{C}_t = \tilde{\mathbf{C}}_t = \mathbf{I}$. But for t smaller P_2 performs better than P_1.

Up to now we discussed uniform grids and therefore the matrix $\mathbf{D}$ is just the identity times a constant and has no influence on the iteration number. This behavior changes if we take a

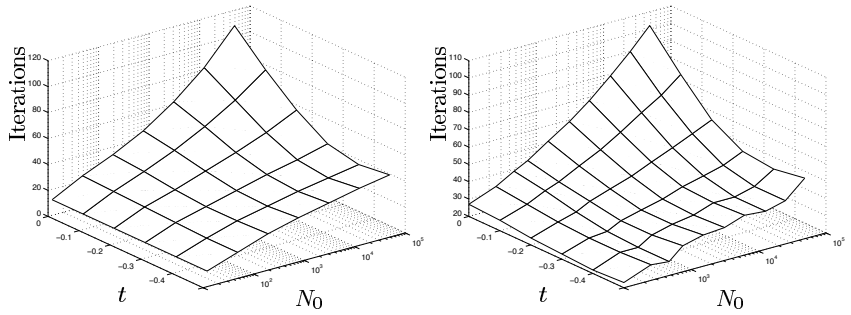

Figure 5.3: Number of GMRes iterations versus number of degrees of freedom and t for G_1 (left) and G_2 (right) with P_3.

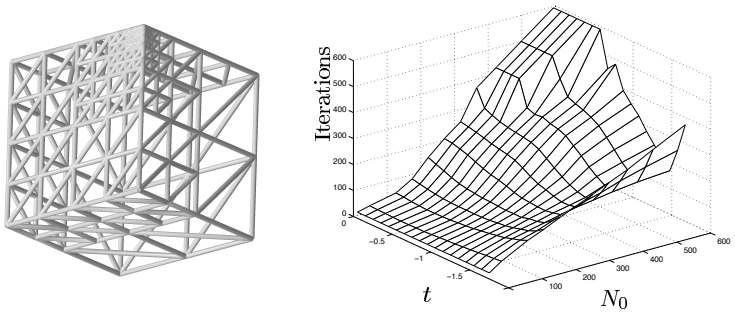

Figure 5.4: G_3, Cube with locally refined mesh (left) and number of GMRes iterations versus number of degrees of freedom and t for G_3 with P_3 (right).

geometry with panels of different sizes. In that case we observed that the iteration number to solve $\mathbf{D}^{-1}\widetilde{\mathbf{A}}\mathbf{D}^{-1}\underline{y} = \mathbf{D}^{-1}\underline{b}$ is substantially larger than for $\widetilde{\mathbf{A}}\underline{x} = \underline{b}$. As a consequence we circumvent the normalization and end up with the problem P_3 where we have to solve

$$\mathbf{A}^{P_3}\underline{y} = \tilde{\mathbf{C}}_t\mathbf{W}\widetilde{\mathbf{A}}\mathbf{W}^\top\tilde{\mathbf{C}}_t\underline{y} = \tilde{\mathbf{C}}_t\mathbf{W}\underline{b}$$

with $\underline{x} = \mathbf{W}^\top\tilde{\mathbf{C}}_t\underline{y}$. For uniform grids the definition of P_3 does not change anything in comparison to P_2 since the normalization is the identity times a constant. This confirms Figure 5.2 and Figure 5.3 where the GMRes iterations versus t and the number of unknowns N_0 for G_1 and G_2 are plotted for P_2 and P_3 respectively.

To test the new preconditioner for strongly locally refined meshes we solve (5.5) on an locally refined grid on the cube.

G_3 This problem consists of a series of adaptive grids on the unit cube. In each step the grid is refined in one corner by one level. The level difference between neighboring patches is restricted to one. The last grid in the series (maximal refinement level 10) is shown in Figure 5.4.

For $t > -0.5$ and $N_0 > 400$ GMRes does not converge and stops after N_0 iteration steps. Decreasing t we achieve convergence as can be seen in Figure 5.4. It seems that for non uniform grids the optimal value of t depends on the quotient of $h_{\min}/h_{\max}$ with $h_{\min}$ the minimal and $h_{\max}$ the maximal mesh size which decreases for larger N_0 in our experiment.

A comparison between P_2 ($t = -0.5$), P_3 ($t = -1.5, -0.5$) and the case without any preconditioning for the adaptively refined cube G_3 can be seen in Figure 5.5. For $h_{\min}/h_{\max}$ small

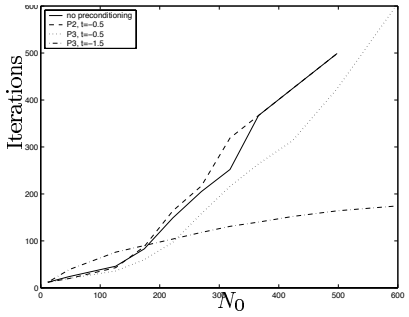

Figure 5.5: Number of GMRes iterations versus number of degrees of freedom for G_3 with P_2 ($t = -0.5$), P_3 ($t = -0.5$ and $t = -1.5$) and without preconditioning.

enough ($N_0 > 400$) GMRes stops after N_0 iterations and does not converge for P_2 and without any preconditioning. With P_3 and choosing t appropriately we get convergence even for the case where $h_{\min}/h_{\max}$ becomes small ($h_{\min}/h_{\max} < 0.002$).

References

[1] R. Beatson, L. Greengard. *A short course on fast multipole methods*, Wavelets, Multilevel Methods and Elliptic PDEs, Oxford Science Publications, 1997.

[2] R. Barret, M. Berry, T. F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, H. van der Vorst. *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM Publ., Philadelphia, 1994.

[3] J.M. Carnicer, W. Dahmen, J.M. Peña. *Local decomposition of refinable spaces and wavelets*, Applied and Computational Harmonic Analysis, **3**, (1996), 127-153.

[4] W. Dahmen. *Wavelet and Multiscale Methods for Operator Equations* Acta Numerica, (1997), 55-228.

[5] W. Dahmen, R. Schneider. *Wavelets on Manifolds - construction and domain decomposition*, SIAM J. Math. Anal., **31**, (1999), 184-230.

[6] W. Dahmen, S. Prössdorf, R. Schneider. *Wavelet approximation methods for pseudo differential equations II: Matrix compression and fast solution*, Adv. Comput. Math. **1**, (1993), 259-335.

[7] W. Dahmen, S. Prössdorf, R. Schneider. *Multiscale methods for pseudo differential equations on smooth closed manifolds*, Wavelet Analysis and its Applications, **5**, (1994), 385-424.

[8] E. Darve. *The Fast Multipole Method: Numerical Implementation.* Journ. Comp. Phys, **160**, (2000), 195-240.

[9] E. Darve. *The Fast Multipole Method (I): Error Analysis and Asymptotic Complexity.* SIAM J. Numer. Anal., **38**, (2000), 98-128.

[10] P. Davis. *Errors of numerical approximation for analytic functions* Journal of Rational Mech. Anal, **2** (1), (1953), 303-313.

[11] S.C. Eisenstat, H.C. Elman, M.H. Schultz. *Variational iterative methods for nonsymmetric systems of linear equations.* SIAM J. Numer. Anal. **20** (920), (1983), 345-357.

[12] L. Greengard, V. Rokhlin.*A new version of the fast multipole method for the Laplace equation in three dimensions*, Acta Numerica **6**, (1997), 229-269, Cambridge University Press.

[13] G.H. Golub, C.F. van Loan. *Matrix Computations*, The Johns Hopkins University Press, 1989.

[14] W. Hackbusch. *Integral equations*, Birkhäuser Publ. Basel, 1995.

[15] W. Hackbusch, Z. P. Nowak. *On the Fast Matrix Multiplication in the Boundary Element Method by Panel Clustering*, Numer. Math. **54**, (1989), 463-491.

[16] G.C. Hsiao, W.L. Wendland. *The Aubin Nitsche lemma for integral equations*, Journal of Integral Equations No. 3, (1981), 299-315.

[17] C. Lage. *Softwareentwicklung zur Randelementmethode: Analyse und Entwurf effizienter Techniken*, Dissertation Universität Kiel, Germany, 1995.

[18] C. Lage, C. Schwab. *Advanced boundary element algorithms*, SAM Research Report, 1999.

[19] Ch. Lage, Ch. Schwab. *Wavelet Galerkin Algorithms for Boundary Integral Equations*, SIAM J. Sci. Comput., **20** (6), (1999), 2195-2222.

[20] P. Oswald. *Multilevel Finite Element Approximation: Theory and Applications*, Teubner Skripte zur Numerik, B. G. Teubner Stuttgart, 1994.

[21] P. Oswald. *Multilevel norms for* $H^{-\frac{1}{2}}$. Computing, (1998).

[22] T. von Petersdorff, Ch. Schwab. *Fully discrete multiscale Galerkin BEM.* In: Multiresolution Analysis and Partial Differential Equations, W. Dahmen, P. Kudila and P. Oswald (eds.). "Wavelet Analysis and its applications", Academic Press, New-York, **6**, (1997), 298-346.

[23] T. von Petersdorff, R. Schneider, C. Schwab. *Multiwavelets for second kind integral equations.* SIAM J. Num. Anal., **34**, (1997), 2212-2227.

[24] T. von Petersdorff, Ch. Schwab. *Fully Discrete Multiscale Galerkin BEM, Wavelet Analysis and its Application*, Academic Press, **6**, (1997), 287-346.

[25] P. Rabinowitz, N. Richter. *New error coefficients for estimating quadrature errors for analytic functions*, Mathematics of Computations, **24** (111), (1970), 561-570.

[26] V. Rokhlin. *Rapid solution of integral equations of classical potential theory.* J. Comput. Physics, **60** (2), (1985), 187-207.

[27] Yousef Saad. *Iterative Methods for Sparse Linear Systems*, PWS Publishing Company, New York, 1996.

[28] S. A. Sauter. *Variable order panel clustering* Computing, 64, (2000), 223-261.

[29] G. Schmidlin, C. Schwab. *Wavelet Galerkin BEM on unstructural meshes by agglomeration.* Report 2000-15, Seminar für Angewandte Mathematik, ETH Zürich.

[30] R. Schneider. *Multiskalen- und Wavelet-Matrixkompression* Advances in Numerical Mathematics, B.G. Teubner Stuttgart, 1998.

[31] W. Sweldens. *The Lifting Scheme: A Custom-Design Construction of Biorthogonal Wavelets*, Appl. Comput. Harmon. Anal., **3** (2), (1996), 186-200.

[32] W. Sweldens. *The Lifting Scheme: A Construction of Second Generation Wavelets*, SIAM J. Math. Anal., **29** (2), (1998), 511-546.

[33] J. Tausch, J White *Multiscale bases for the sparse representation of boundary integral operators on complex geometry*, SMU Math Report 2000-01.

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